



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:31 am BST

PDB ID : 4G9I  
Title : Crystal structure of T.kodakarensis HypF  
Authors : Tominaga, T.; Watanabe, S.; Matsumi, R.; Atomi, H.; Imanaka, T.; Miki, K.  
Deposited on : 2012-07-24  
Resolution : 4.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

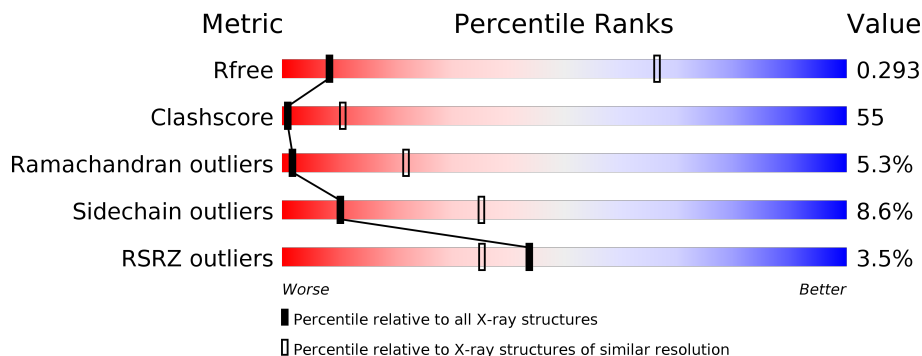
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1055 (5.20-3.80)                                      |
| Clashscore            | 141614                      | 1123 (5.20-3.80)                                      |
| Ramachandran outliers | 138981                      | 1069 (5.20-3.80)                                      |
| Sidechain outliers    | 138945                      | 1050 (5.20-3.80)                                      |
| RSRZ outliers         | 127900                      | 1101 (5.30-3.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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     | 772    |                  |
| 1   | B     | 772    |                  |
| 1   | C     | 772    |                  |
| 1   | D     | 772    |                  |
| 1   | E     | 772    |                  |
| 1   | F     | 772    |                  |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 36065 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 Hydrogenase maturation protein HypF.

| Mol | Chain | Residues | Atoms         |           |           |           |         | ZeroOcc  | AltConf | Trace |    |
|-----|-------|----------|---------------|-----------|-----------|-----------|---------|----------|---------|-------|----|
|     |       |          | Total         | C         | N         | O         | S       |          |         |       | Se |
| 1   | A     | 766      | Total<br>6032 | C<br>3862 | N<br>1028 | O<br>1113 | S<br>11 | Se<br>18 | 0       | 0     | 0  |
| 1   | B     | 762      | Total<br>6008 | C<br>3847 | N<br>1024 | O<br>1108 | S<br>11 | Se<br>18 | 0       | 0     | 0  |
| 1   | C     | 756      | Total<br>5964 | C<br>3819 | N<br>1017 | O<br>1100 | S<br>11 | Se<br>17 | 0       | 0     | 0  |
| 1   | D     | 765      | Total<br>6027 | C<br>3859 | N<br>1027 | O<br>1112 | S<br>11 | Se<br>18 | 0       | 0     | 0  |
| 1   | E     | 762      | Total<br>6008 | C<br>3847 | N<br>1024 | O<br>1108 | S<br>11 | Se<br>18 | 0       | 0     | 0  |
| 1   | F     | 762      | Total<br>6008 | C<br>3847 | N<br>1024 | O<br>1108 | S<br>11 | Se<br>18 | 0       | 0     | 0  |

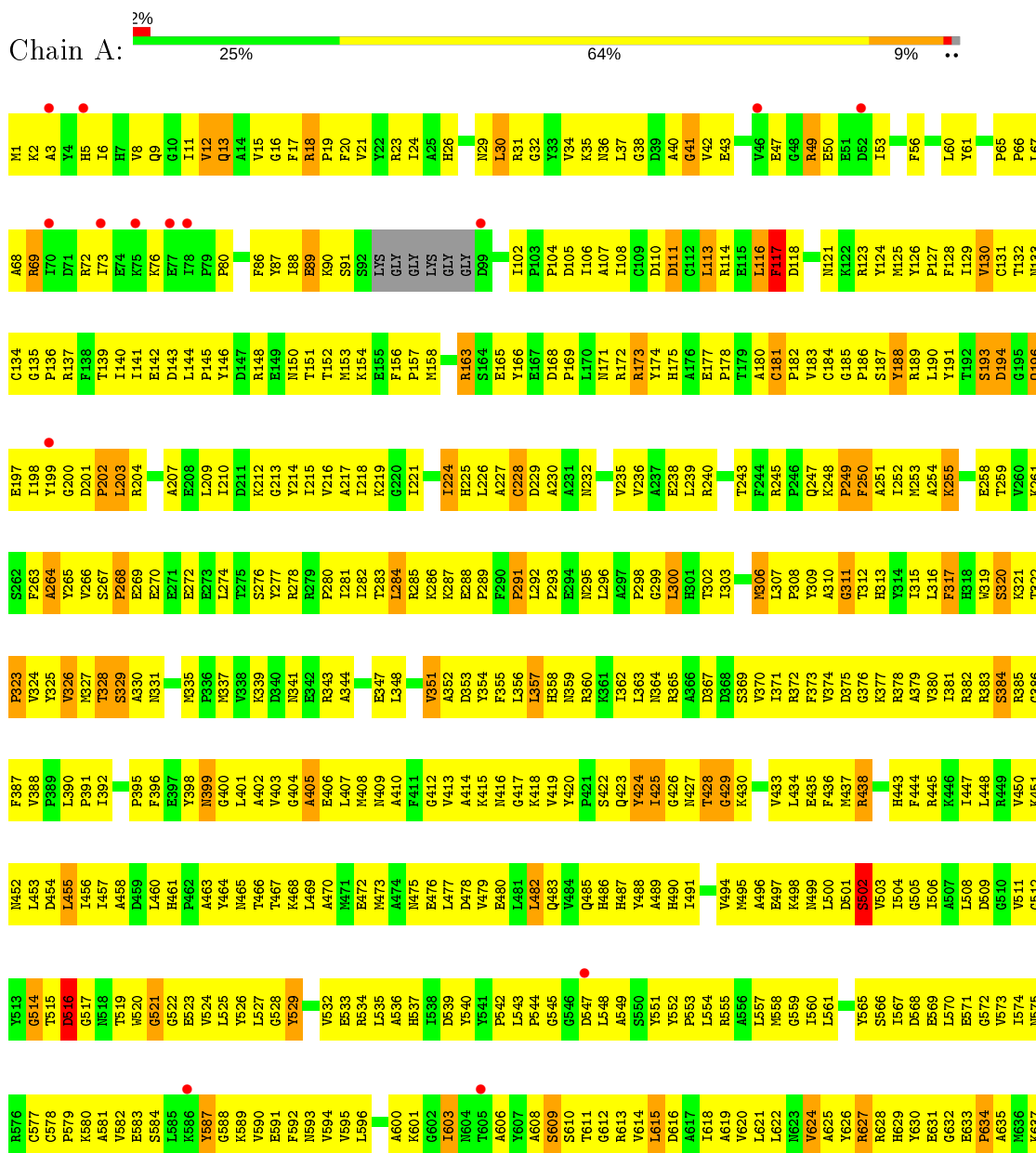
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

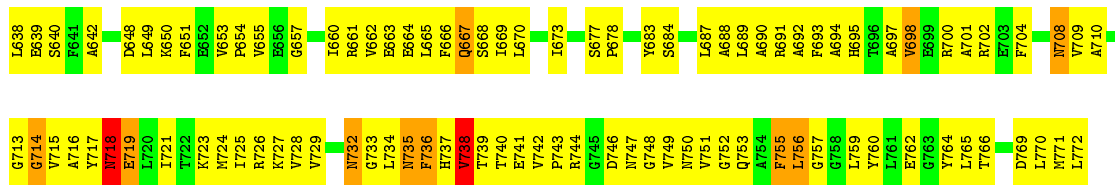
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | D     | 3        | Total<br>3 | Zn<br>3 | 0       | 0       |
| 2   | E     | 3        | Total<br>3 | Zn<br>3 | 0       | 0       |
| 2   | B     | 3        | Total<br>3 | Zn<br>3 | 0       | 0       |
| 2   | C     | 3        | Total<br>3 | Zn<br>3 | 0       | 0       |
| 2   | A     | 3        | Total<br>3 | Zn<br>3 | 0       | 0       |
| 2   | F     | 3        | Total<br>3 | Zn<br>3 | 0       | 0       |

### 3 Residue-property plots

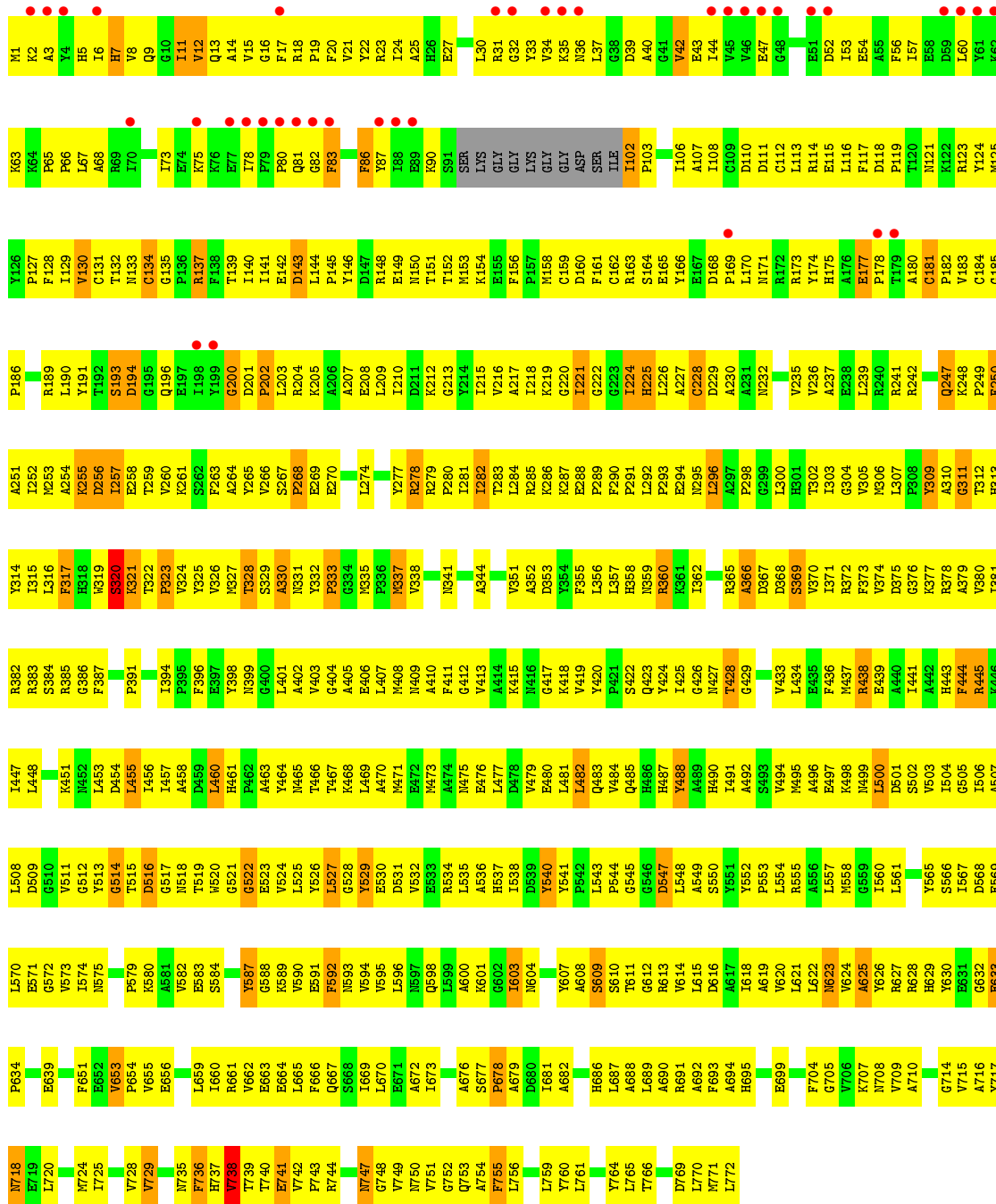
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Hydrogenase maturation protein HypF

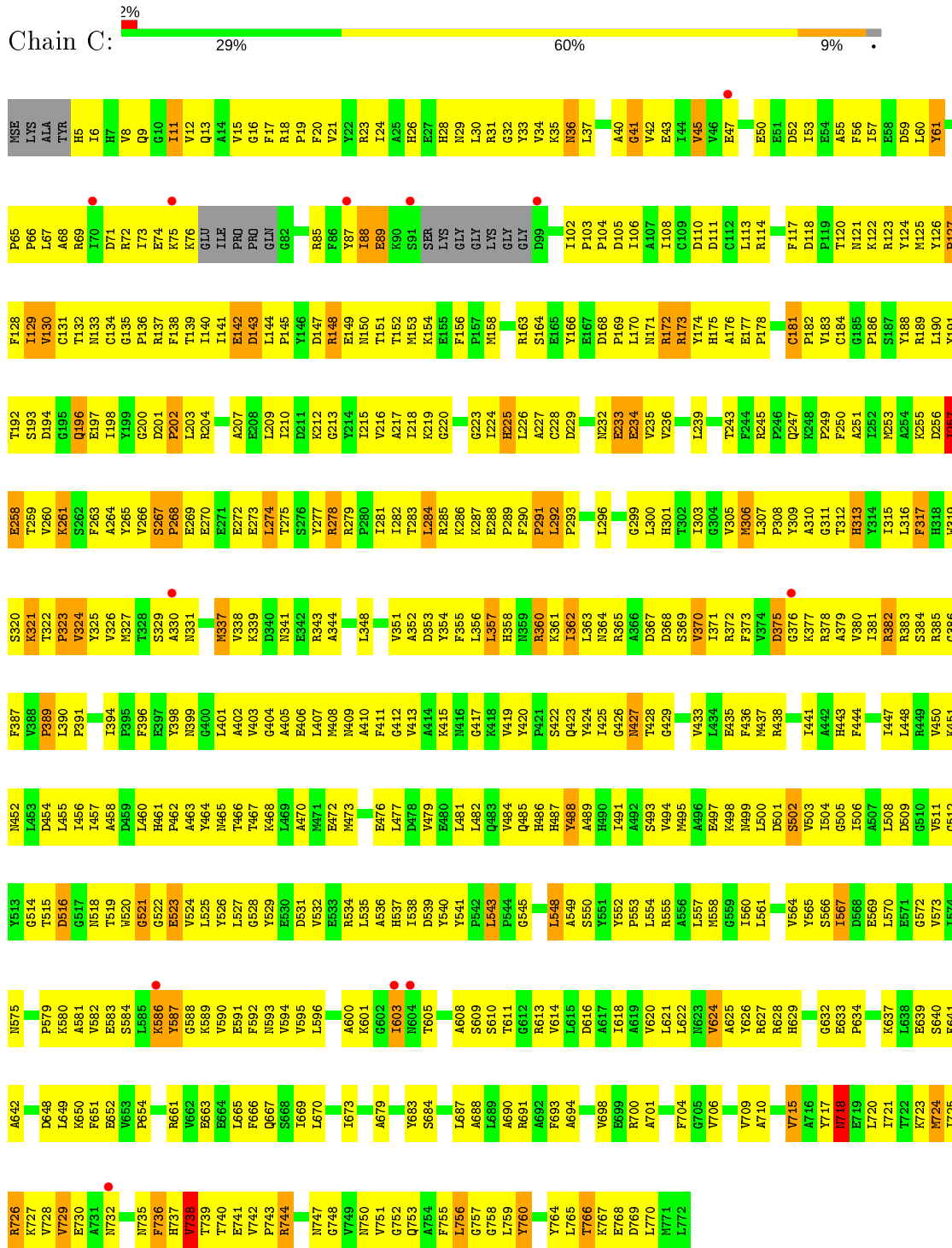




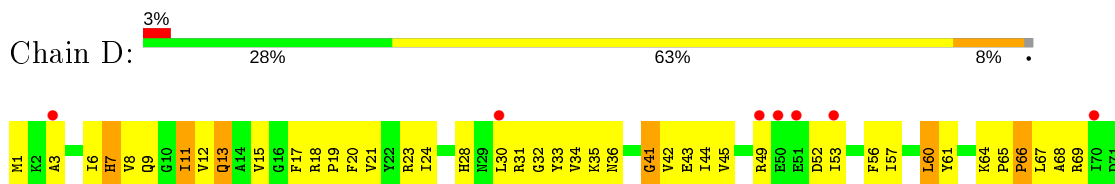
• Molecule 1: Hydrogenase maturation protein HypF



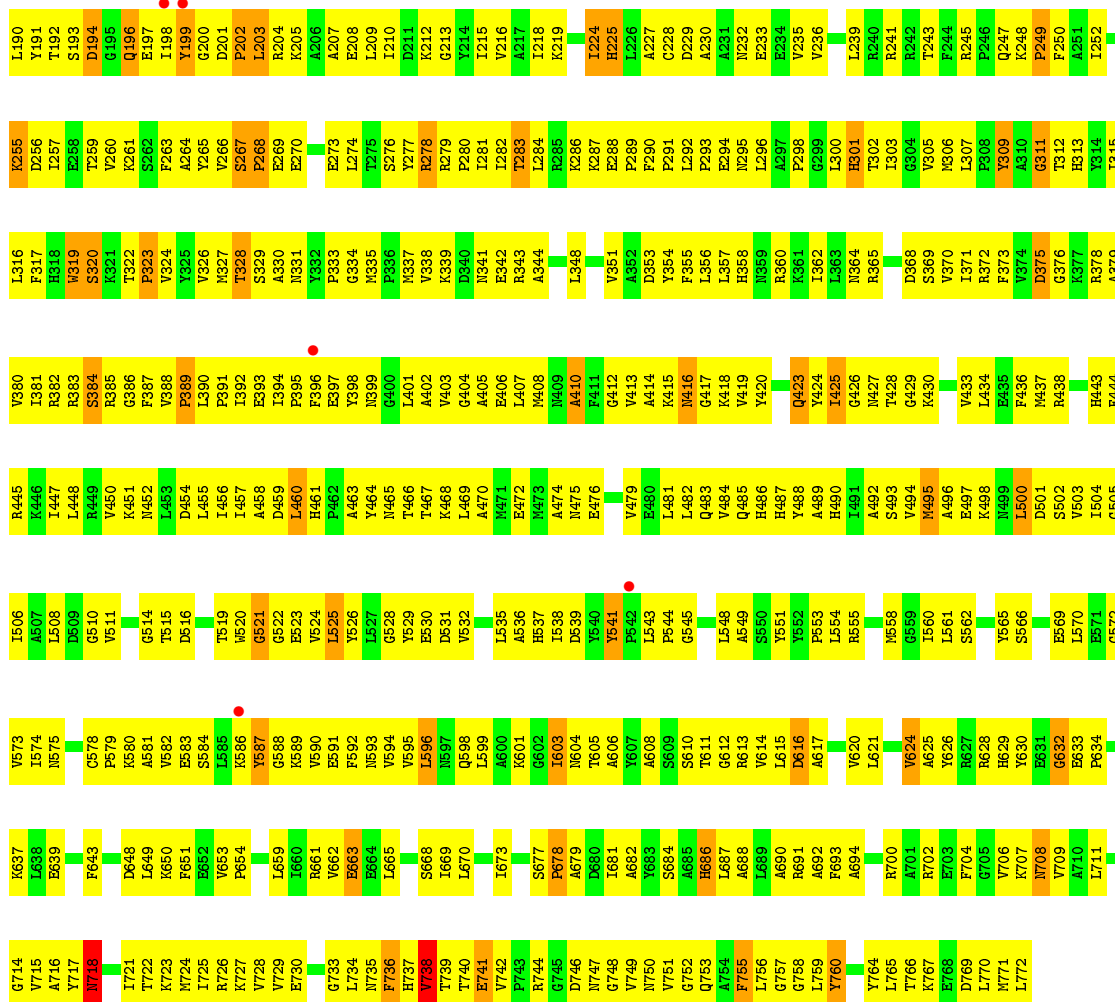
• Molecule 1: Hydrogenase maturation protein HypF



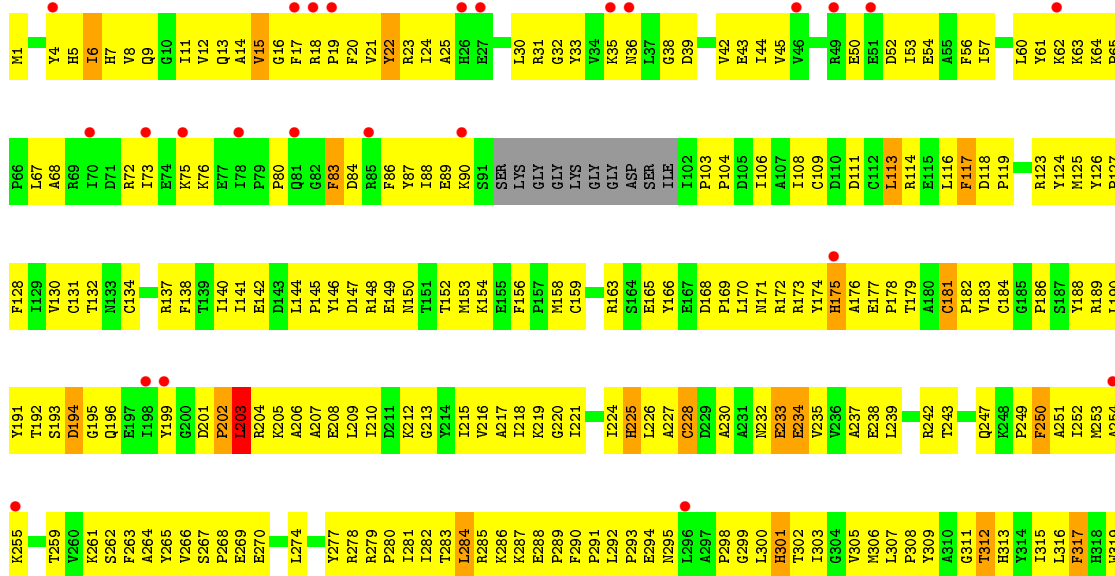
• Molecule 1: Hydrogenase maturation protein HypF



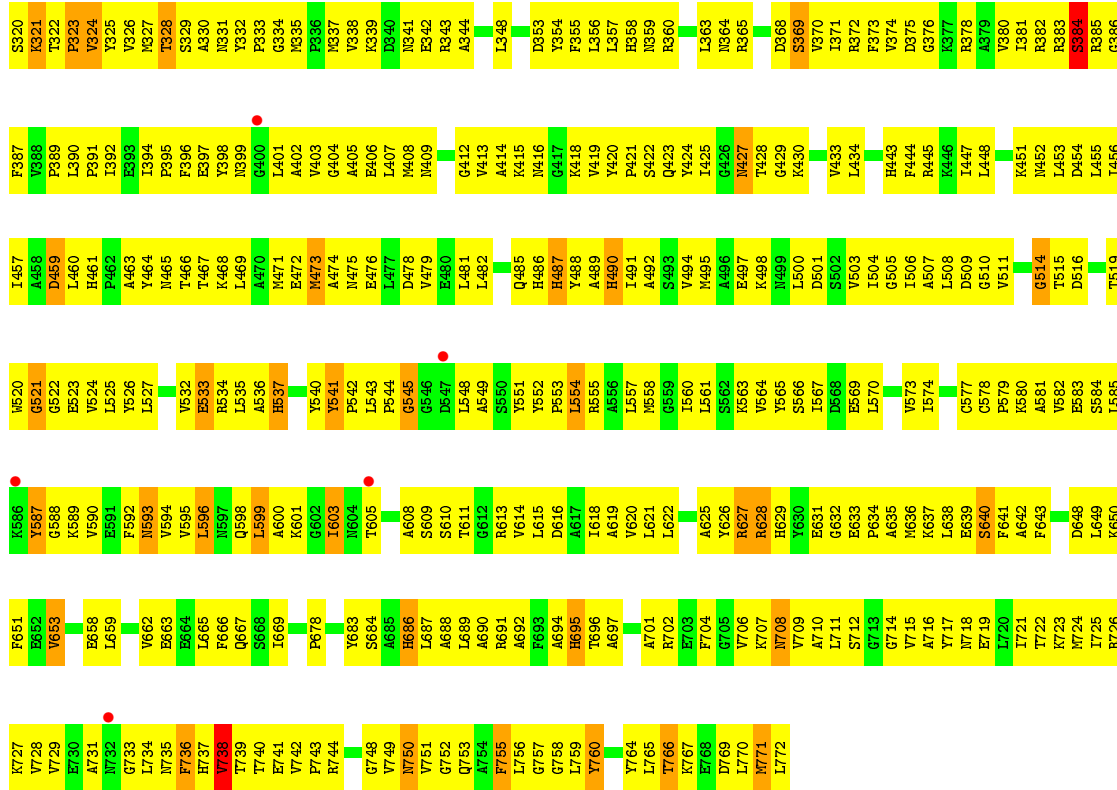




● Molecule 1: Hydrogenase maturation protein HypF







## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 65 2 2  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 265.81Å 265.81Å 693.71Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)  | 15.00 – 4.50<br>49.77 – 4.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.5 (15.00-4.50)<br>94.9 (49.77-4.50)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.17  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.46 (at 4.45Å)   | Xtrriage         |
| Refinement program  | CNS 1.3   | Depositor        |
| R, $R_{free}$   | 0.279 , 0.300<br>0.298 , 0.293                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4326 reflections (5.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 143.9   | Xtrriage         |
| Anisotropy  | 0.170   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 153.6  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.83  | EDS              |
| Total number of atoms   | 36065   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 186.0   | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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:  
ZN

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     | 0.25         | 0/6151  | 0.49        | 0/8308         |
| 1   | B     | 0.25         | 0/6127  | 0.49        | 1/8275 (0.0%)  |
| 1   | C     | 0.25         | 0/6080  | 0.49        | 0/8208         |
| 1   | D     | 0.25         | 0/6146  | 0.49        | 0/8301         |
| 1   | E     | 0.25         | 0/6127  | 0.49        | 0/8275         |
| 1   | F     | 0.25         | 0/6127  | 0.50        | 0/8275         |
| All | All   | 0.25         | 0/36758 | 0.49        | 1/49642 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | B     | 200 | GLY  | N-CA-C | 5.11 | 125.88      | 113.10   |

There are no chirality outliers.

There are no planarity outliers.

### 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     | 6032  | 0        | 5969     | 684     | 1            |
| 1   | B     | 6008  | 0        | 5954     | 671     | 0            |
| 1   | C     | 5964  | 0        | 5909     | 669     | 0            |
| 1   | D     | 6027  | 0        | 5970     | 674     | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 6008  | 0        | 5954     | 616     | 0            |
| 1   | F     | 6008  | 0        | 5955     | 667     | 0            |
| 2   | A     | 3     | 0        | 0        | 0       | 0            |
| 2   | B     | 3     | 0        | 0        | 0       | 0            |
| 2   | C     | 3     | 0        | 0        | 0       | 0            |
| 2   | D     | 3     | 0        | 0        | 0       | 0            |
| 2   | E     | 3     | 0        | 0        | 0       | 0            |
| 2   | F     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 36065 | 0        | 35711    | 3925    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

All (3925) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:11:ILE:HG21  | 1:A:69:ARG:H     | 1.24                     | 1.02              |
| 1:D:9:GLN:HE21   | 1:D:41:GLY:HA2   | 1.17                     | 1.02              |
| 1:D:485:GLN:HE21 | 1:D:487:HIS:H    | 1.04                     | 1.01              |
| 1:D:451:LYS:HA   | 1:D:477:LEU:HD21 | 1.41                     | 0.99              |
| 1:F:394:ILE:HD11 | 1:F:419:VAL:HB   | 1.41                     | 0.99              |
| 1:D:288:GLU:HB3  | 1:D:289:PRO:HD3  | 1.45                     | 0.98              |
| 1:C:198:ILE:HG13 | 1:D:122:LYS:HD3  | 1.39                     | 0.98              |
| 1:B:485:GLN:HE21 | 1:B:487:HIS:H    | 1.04                     | 0.98              |
| 1:B:57:ILE:HG13  | 1:B:75:LYS:HZ3   | 1.28                     | 0.98              |
| 1:B:456:ILE:HG22 | 1:B:457:ILE:H    | 1.26                     | 0.98              |
| 1:A:268:PRO:HG2  | 1:A:378:ARG:HH22 | 1.28                     | 0.97              |
| 1:A:485:GLN:HE21 | 1:A:487:HIS:H    | 1.10                     | 0.97              |
| 1:B:225:HIS:HA   | 1:B:330:ALA:HB2  | 1.44                     | 0.97              |
| 1:D:369:SER:H    | 1:D:385:ARG:HB2  | 1.28                     | 0.97              |
| 1:E:39:ASP:HB3   | 1:E:144:LEU:HD13 | 1.45                     | 0.97              |
| 1:F:485:GLN:HE21 | 1:F:487:HIS:H    | 1.01                     | 0.97              |
| 1:F:288:GLU:HB3  | 1:F:289:PRO:HD3  | 1.46                     | 0.96              |
| 1:D:88:ILE:HG22  | 1:D:89:GLU:H     | 1.31                     | 0.96              |
| 1:E:127:PRO:HB3  | 1:E:312:THR:HG22 | 1.47                     | 0.96              |
| 1:C:127:PRO:HB3  | 1:C:312:THR:HG22 | 1.46                     | 0.96              |
| 1:B:288:GLU:HB3  | 1:B:289:PRO:HD3  | 1.47                     | 0.95              |
| 1:A:587:TYR:HD1  | 1:A:588:GLY:H    | 1.14                     | 0.95              |
| 1:A:557:LEU:HD21 | 1:A:621:LEU:HD13 | 1.49                     | 0.95              |
| 1:C:191:TYR:HB2  | 1:C:355:PHE:HB2  | 1.47                     | 0.95              |
| 1:A:475:ASN:HD22 | 1:B:591:GLU:HG2  | 1.32                     | 0.94              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:181:CYS:SG   | 1:A:183:VAL:HG22 | 2.07                     | 0.94              |
| 1:E:485:GLN:HE21 | 1:E:487:HIS:H    | 0.96                     | 0.94              |
| 1:A:11:ILE:HG12  | 1:A:68:ALA:HA    | 1.49                     | 0.94              |
| 1:E:369:SER:H    | 1:E:385:ARG:HB2  | 1.31                     | 0.94              |
| 1:B:394:ILE:HD11 | 1:B:419:VAL:HB   | 1.47                     | 0.94              |
| 1:F:216:VAL:HB   | 1:F:354:TYR:HB2  | 1.50                     | 0.94              |
| 1:A:379:ALA:HB3  | 1:A:744:ARG:HH11 | 1.31                     | 0.94              |
| 1:E:169:PRO:HG2  | 1:E:170:LEU:HD12 | 1.48                     | 0.94              |
| 1:C:288:GLU:HB2  | 1:C:289:PRO:HD3  | 1.47                     | 0.93              |
| 1:A:287:LYS:HG3  | 1:A:289:PRO:HD2  | 1.49                     | 0.93              |
| 1:D:127:PRO:HB3  | 1:D:312:THR:HG22 | 1.48                     | 0.93              |
| 1:B:268:PRO:HG2  | 1:B:378:ARG:HH22 | 1.31                     | 0.93              |
| 1:C:519:THR:HB   | 1:C:608:ALA:HA   | 1.51                     | 0.93              |
| 1:D:111:ASP:HB2  | 1:D:172:ARG:HH22 | 1.34                     | 0.93              |
| 1:E:394:ILE:HD11 | 1:E:419:VAL:HB   | 1.51                     | 0.93              |
| 1:B:612:GLY:HA2  | 1:B:615:LEU:HD12 | 1.51                     | 0.93              |
| 1:C:504:ILE:HB   | 1:C:709:VAL:HG12 | 1.51                     | 0.93              |
| 1:A:288:GLU:HB3  | 1:A:289:PRO:HD3  | 1.48                     | 0.92              |
| 1:F:207:ALA:HB1  | 1:F:320:SER:HB2  | 1.49                     | 0.92              |
| 1:A:553:PRO:HB2  | 1:A:620:VAL:HG21 | 1.50                     | 0.92              |
| 1:F:190:LEU:HD21 | 1:F:206:ALA:HB2  | 1.50                     | 0.92              |
| 1:D:11:ILE:HG12  | 1:D:68:ALA:HA    | 1.51                     | 0.92              |
| 1:C:286:LYS:HD2  | 1:C:303:ILE:HD11 | 1.51                     | 0.92              |
| 1:F:219:LYS:HD3  | 1:F:358:HIS:H    | 1.33                     | 0.92              |
| 1:A:108:ILE:HG12 | 1:A:310:ALA:HA   | 1.52                     | 0.92              |
| 1:E:738:VAL:HG23 | 1:E:744:ARG:HG2  | 1.51                     | 0.92              |
| 1:A:380:VAL:HG12 | 1:A:381:ILE:H    | 1.34                     | 0.91              |
| 1:E:149:GLU:HA   | 1:E:154:LYS:HG2  | 1.49                     | 0.91              |
| 1:B:232:ASN:HB3  | 1:B:235:VAL:HG22 | 1.52                     | 0.91              |
| 1:B:39:ASP:HB3   | 1:B:144:LEU:HD13 | 1.52                     | 0.90              |
| 1:B:14:ALA:HB3   | 1:B:103:PRO:HG3  | 1.53                     | 0.90              |
| 1:D:111:ASP:HB3  | 1:D:172:ARG:HH12 | 1.33                     | 0.90              |
| 1:E:288:GLU:HB3  | 1:E:289:PRO:HD3  | 1.52                     | 0.90              |
| 1:F:369:SER:H    | 1:F:385:ARG:HB2  | 1.35                     | 0.90              |
| 1:F:508:LEU:HD22 | 1:F:611:THR:HG21 | 1.51                     | 0.90              |
| 1:E:191:TYR:HB2  | 1:E:355:PHE:HB2  | 1.54                     | 0.89              |
| 1:A:628:ARG:NH2  | 1:A:632:GLY:H    | 1.69                     | 0.89              |
| 1:F:19:PRO:HG2   | 1:F:132:THR:HG21 | 1.53                     | 0.89              |
| 1:E:287:LYS:HG3  | 1:E:289:PRO:HD2  | 1.51                     | 0.89              |
| 1:B:149:GLU:HA   | 1:B:154:LYS:HG2  | 1.54                     | 0.89              |
| 1:E:494:VAL:HG22 | 1:E:738:VAL:HG22 | 1.54                     | 0.89              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:106:ILE:HG23 | 1:B:277:TYR:HB2  | 1.54                     | 0.89              |
| 1:A:230:ALA:HB2  | 1:A:326:VAL:HG23 | 1.55                     | 0.89              |
| 1:B:615:LEU:HA   | 1:B:618:ILE:HD12 | 1.55                     | 0.89              |
| 1:D:331:ASN:HD22 | 1:D:337:MSE:HA   | 1.36                     | 0.89              |
| 1:D:543:LEU:H    | 1:D:543:LEU:HD23 | 1.37                     | 0.89              |
| 1:C:281:ILE:HB   | 1:C:370:VAL:HG12 | 1.52                     | 0.89              |
| 1:A:219:LYS:HD3  | 1:A:358:HIS:H    | 1.37                     | 0.88              |
| 1:D:281:ILE:HB   | 1:D:370:VAL:HG12 | 1.54                     | 0.88              |
| 1:D:458:ALA:HB1  | 1:D:467:THR:HG22 | 1.55                     | 0.88              |
| 1:F:190:LEU:HG   | 1:F:202:PRO:HB3  | 1.55                     | 0.88              |
| 1:E:153:MSE:HE1  | 1:E:360:ARG:HD2  | 1.55                     | 0.88              |
| 1:E:765:LEU:HD21 | 1:E:770:LEU:HD21 | 1.55                     | 0.88              |
| 1:C:369:SER:H    | 1:C:385:ARG:HB2  | 1.38                     | 0.88              |
| 1:F:282:ILE:HD12 | 1:F:371:ILE:HG23 | 1.53                     | 0.87              |
| 1:D:106:ILE:HG23 | 1:D:277:TYR:HB2  | 1.56                     | 0.87              |
| 1:F:261:LYS:NZ   | 1:F:266:VAL:HB   | 1.90                     | 0.87              |
| 1:F:219:LYS:HA   | 1:F:224:ILE:HG12 | 1.56                     | 0.87              |
| 1:F:281:ILE:HB   | 1:F:370:VAL:HG12 | 1.56                     | 0.87              |
| 1:C:371:ILE:HD12 | 1:C:380:VAL:HG22 | 1.57                     | 0.87              |
| 1:E:690:ALA:HB1  | 1:E:725:ILE:HG13 | 1.55                     | 0.87              |
| 1:F:653:VAL:HG13 | 1:F:692:ALA:HB3  | 1.54                     | 0.87              |
| 1:D:566:SER:H    | 1:D:569:GLU:HB2  | 1.39                     | 0.86              |
| 1:E:485:GLN:NE2  | 1:E:487:HIS:H    | 1.73                     | 0.86              |
| 1:F:380:VAL:HG23 | 1:F:740:THR:HA   | 1.57                     | 0.86              |
| 1:A:456:ILE:HG22 | 1:A:457:ILE:H    | 1.40                     | 0.86              |
| 1:C:207:ALA:HB1  | 1:C:320:SER:HB2  | 1.54                     | 0.86              |
| 1:C:331:ASN:HD22 | 1:C:337:MSE:HA   | 1.41                     | 0.86              |
| 1:D:370:VAL:HG22 | 1:D:382:ARG:HD2  | 1.57                     | 0.86              |
| 1:D:9:GLN:HB2    | 1:D:72:ARG:HD2   | 1.56                     | 0.86              |
| 1:B:128:PHE:HB3  | 1:B:360:ARG:HH22 | 1.38                     | 0.86              |
| 1:E:485:GLN:HE21 | 1:E:487:HIS:N    | 1.73                     | 0.86              |
| 1:A:371:ILE:HB   | 1:A:380:VAL:HG13 | 1.56                     | 0.86              |
| 1:B:249:PRO:HG3  | 1:B:300:LEU:HD13 | 1.58                     | 0.86              |
| 1:F:615:LEU:HD12 | 1:F:638:LEU:HD23 | 1.56                     | 0.86              |
| 1:C:502:SER:HB3  | 1:C:528:GLY:HA2  | 1.58                     | 0.86              |
| 1:C:485:GLN:HG3  | 1:C:488:TYR:H    | 1.41                     | 0.85              |
| 1:D:102:ILE:HD11 | 1:D:144:LEU:HG   | 1.58                     | 0.85              |
| 1:A:201:ASP:N    | 1:A:202:PRO:HD2  | 1.91                     | 0.85              |
| 1:A:281:ILE:HG12 | 1:A:306:MSE:HG3  | 1.55                     | 0.85              |
| 1:E:543:LEU:HD23 | 1:E:543:LEU:H    | 1.40                     | 0.85              |
| 1:C:219:LYS:HA   | 1:C:224:ILE:HB   | 1.58                     | 0.85              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:458:ALA:HB1  | 1:A:467:THR:HG22 | 1.58                     | 0.85              |
| 1:B:544:PRO:HB2  | 1:B:555:ARG:HH21 | 1.42                     | 0.85              |
| 1:D:687:LEU:HB3  | 1:D:724:MSE:HE2  | 1.56                     | 0.85              |
| 1:C:153:MSE:HE1  | 1:C:360:ARG:HD3  | 1.57                     | 0.85              |
| 1:F:149:GLU:HA   | 1:F:154:LYS:HG2  | 1.57                     | 0.85              |
| 1:B:765:LEU:HD21 | 1:B:770:LEU:HD21 | 1.59                     | 0.85              |
| 1:B:369:SER:H    | 1:B:385:ARG:HB2  | 1.41                     | 0.85              |
| 1:C:543:LEU:HD23 | 1:C:543:LEU:H    | 1.41                     | 0.85              |
| 1:D:374:VAL:HG21 | 1:D:744:ARG:HH22 | 1.41                     | 0.85              |
| 1:F:5:HIS:HB3    | 1:F:76:LYS:HB2   | 1.59                     | 0.84              |
| 1:E:281:ILE:HB   | 1:E:370:VAL:HG12 | 1.58                     | 0.84              |
| 1:F:589:LYS:HG3  | 1:F:590:VAL:H    | 1.42                     | 0.84              |
| 1:C:485:GLN:HE22 | 1:C:514:GLY:HA2  | 1.42                     | 0.84              |
| 1:D:181:CYS:SG   | 1:D:183:VAL:HG22 | 2.16                     | 0.84              |
| 1:B:191:TYR:HB2  | 1:B:355:PHE:HB2  | 1.57                     | 0.84              |
| 1:A:404:GLY:HA2  | 1:A:753:GLN:HE22 | 1.42                     | 0.84              |
| 1:A:589:LYS:HG3  | 1:A:590:VAL:H    | 1.40                     | 0.84              |
| 1:C:282:ILE:HD12 | 1:C:371:ILE:HG23 | 1.59                     | 0.84              |
| 1:C:261:LYS:NZ   | 1:C:266:VAL:HB   | 1.93                     | 0.84              |
| 1:D:247:GLN:HG3  | 1:D:298:PRO:HG2  | 1.59                     | 0.84              |
| 1:A:425:ILE:HD12 | 1:A:437:MSE:HE2  | 1.59                     | 0.84              |
| 1:A:524:VAL:HG22 | 1:A:536:ALA:HB3  | 1.60                     | 0.84              |
| 1:E:270:GLU:HB2  | 1:E:373:PHE:HE2  | 1.42                     | 0.84              |
| 1:A:163:ARG:HH11 | 1:A:163:ARG:HB2  | 1.42                     | 0.83              |
| 1:C:258:GLU:HG3  | 1:C:259:THR:N    | 1.93                     | 0.83              |
| 1:D:233:GLU:HB2  | 1:D:295:ASN:HD21 | 1.40                     | 0.83              |
| 1:F:265:TYR:HE2  | 1:F:287:LYS:HD2  | 1.42                     | 0.83              |
| 1:C:457:ILE:HG21 | 1:C:753:GLN:HB3  | 1.60                     | 0.83              |
| 1:A:491:ILE:HG23 | 1:A:527:LEU:HD11 | 1.60                     | 0.83              |
| 1:B:281:ILE:HB   | 1:B:370:VAL:HG12 | 1.60                     | 0.83              |
| 1:C:409:ASN:HD22 | 1:C:425:ILE:HD11 | 1.43                     | 0.83              |
| 1:A:267:SER:HB2  | 1:A:270:GLU:HB2  | 1.59                     | 0.83              |
| 1:D:225:HIS:HA   | 1:D:330:ALA:HB2  | 1.60                     | 0.83              |
| 1:E:425:ILE:HD12 | 1:E:437:MSE:HE2  | 1.60                     | 0.83              |
| 1:F:57:ILE:HG13  | 1:F:75:LYS:NZ    | 1.94                     | 0.83              |
| 1:E:18:ARG:HB2   | 1:E:19:PRO:HD3   | 1.61                     | 0.83              |
| 1:D:506:ILE:HD11 | 1:D:694:ALA:HA   | 1.61                     | 0.82              |
| 1:A:404:GLY:HA2  | 1:A:753:GLN:NE2  | 1.94                     | 0.82              |
| 1:B:587:TYR:HD1  | 1:B:588:GLY:H    | 1.27                     | 0.82              |
| 1:F:225:HIS:HA   | 1:F:330:ALA:HB2  | 1.59                     | 0.82              |
| 1:E:210:ILE:HD11 | 1:E:228:CYS:HA   | 1.60                     | 0.82              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:494:VAL:HG22 | 1:B:738:VAL:HG22 | 1.59                     | 0.82              |
| 1:D:1:MSE:HB3    | 1:D:80:PRO:HD2   | 1.61                     | 0.82              |
| 1:D:519:THR:HB   | 1:D:608:ALA:HA   | 1.60                     | 0.82              |
| 1:E:20:PHE:HD2   | 1:E:23:ARG:HH21  | 1.26                     | 0.82              |
| 1:F:711:LEU:HD13 | 1:F:725:ILE:HG21 | 1.61                     | 0.82              |
| 1:B:451:LYS:HA   | 1:B:477:LEU:HD21 | 1.61                     | 0.82              |
| 1:E:380:VAL:HG23 | 1:E:740:THR:HA   | 1.61                     | 0.82              |
| 1:C:470:ALA:HB1  | 1:C:481:LEU:HD11 | 1.61                     | 0.82              |
| 1:E:181:CYS:SG   | 1:E:183:VAL:HG22 | 2.19                     | 0.82              |
| 1:E:249:PRO:HG3  | 1:E:300:LEU:HD13 | 1.60                     | 0.82              |
| 1:A:281:ILE:HB   | 1:A:370:VAL:HG12 | 1.60                     | 0.82              |
| 1:B:380:VAL:HG23 | 1:B:740:THR:HA   | 1.61                     | 0.82              |
| 1:E:201:ASP:N    | 1:E:202:PRO:HD2  | 1.94                     | 0.82              |
| 1:B:331:ASN:HD22 | 1:B:337:MSE:HA   | 1.45                     | 0.81              |
| 1:C:215:ILE:HD12 | 1:C:226:LEU:HD23 | 1.62                     | 0.81              |
| 1:A:495:MSE:SE   | 1:A:527:LEU:HD13 | 2.30                     | 0.81              |
| 1:E:331:ASN:HD22 | 1:E:337:MSE:HA   | 1.45                     | 0.81              |
| 1:C:587:TYR:HD1  | 1:C:588:GLY:H    | 1.27                     | 0.81              |
| 1:B:457:ILE:HG21 | 1:B:753:GLN:HB3  | 1.61                     | 0.81              |
| 1:D:544:PRO:HG2  | 1:D:555:ARG:HB3  | 1.62                     | 0.81              |
| 1:D:230:ALA:HB1  | 1:D:296:LEU:HD21 | 1.62                     | 0.81              |
| 1:F:554:LEU:HD11 | 1:F:579:PRO:HB2  | 1.60                     | 0.81              |
| 1:F:419:VAL:HG11 | 1:F:751:VAL:HG23 | 1.62                     | 0.81              |
| 1:C:103:PRO:HG2  | 1:C:137:ARG:HD2  | 1.60                     | 0.81              |
| 1:E:589:LYS:HG3  | 1:E:590:VAL:H    | 1.45                     | 0.81              |
| 1:A:457:ILE:HG21 | 1:A:753:GLN:HB3  | 1.63                     | 0.81              |
| 1:A:625:ALA:HB2  | 1:A:637:LYS:HD3  | 1.63                     | 0.81              |
| 1:B:247:GLN:HE21 | 1:B:298:PRO:HG2  | 1.44                     | 0.81              |
| 1:F:765:LEU:HD21 | 1:F:770:LEU:HD21 | 1.61                     | 0.81              |
| 1:B:374:VAL:HG21 | 1:B:744:ARG:HH22 | 1.45                     | 0.81              |
| 1:B:485:GLN:NE2  | 1:B:487:HIS:H    | 1.80                     | 0.81              |
| 1:C:6:ILE:HG22   | 1:C:8:VAL:HG23   | 1.63                     | 0.81              |
| 1:F:247:GLN:HG3  | 1:F:298:PRO:HG2  | 1.62                     | 0.81              |
| 1:F:504:ILE:HB   | 1:F:709:VAL:HG12 | 1.63                     | 0.81              |
| 1:B:485:GLN:HG3  | 1:B:488:TYR:H    | 1.46                     | 0.80              |
| 1:E:484:VAL:HG12 | 1:E:770:LEU:HD13 | 1.63                     | 0.80              |
| 1:C:225:HIS:HA   | 1:C:330:ALA:HB2  | 1.63                     | 0.80              |
| 1:A:127:PRO:HB3  | 1:A:312:THR:HG22 | 1.62                     | 0.80              |
| 1:A:191:TYR:HB2  | 1:A:355:PHE:HB2  | 1.64                     | 0.80              |
| 1:B:425:ILE:HD12 | 1:B:437:MSE:HE2  | 1.61                     | 0.80              |
| 1:D:587:TYR:HD1  | 1:D:588:GLY:H    | 1.24                     | 0.80              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:580:LYS:HG3  | 1:F:593:ASN:HD22 | 1.44                     | 0.80              |
| 1:F:521:GLY:HA3  | 1:F:610:SER:HA   | 1.63                     | 0.80              |
| 1:B:519:THR:HB   | 1:B:608:ALA:HA   | 1.64                     | 0.80              |
| 1:B:451:LYS:HG3  | 1:B:477:LEU:HD11 | 1.62                     | 0.80              |
| 1:C:181:CYS:SG   | 1:C:183:VAL:HG22 | 2.22                     | 0.80              |
| 1:C:458:ALA:HB1  | 1:C:467:THR:HG22 | 1.63                     | 0.80              |
| 1:E:711:LEU:HD13 | 1:E:725:ILE:HG21 | 1.64                     | 0.80              |
| 1:C:201:ASP:N    | 1:C:202:PRO:HD2  | 1.97                     | 0.79              |
| 1:D:249:PRO:HG3  | 1:D:300:LEU:HD13 | 1.64                     | 0.79              |
| 1:F:545:GLY:HA3  | 1:F:548:LEU:HB2  | 1.64                     | 0.79              |
| 1:F:691:ARG:HD3  | 1:F:724:MSE:HE3  | 1.64                     | 0.79              |
| 1:C:253:MSE:HG2  | 1:C:317:PHE:HE1  | 1.45                     | 0.79              |
| 1:C:269:GLU:HB2  | 1:C:378:ARG:CZ   | 2.12                     | 0.79              |
| 1:C:485:GLN:HB3  | 1:C:488:TYR:HB2  | 1.64                     | 0.79              |
| 1:B:163:ARG:HB2  | 1:B:163:ARG:HH11 | 1.47                     | 0.79              |
| 1:F:371:ILE:HD12 | 1:F:380:VAL:HG22 | 1.64                     | 0.79              |
| 1:E:111:ASP:HB3  | 1:E:172:ARG:HH22 | 1.48                     | 0.79              |
| 1:F:404:GLY:HA2  | 1:F:753:GLN:HE22 | 1.47                     | 0.79              |
| 1:B:282:ILE:HD12 | 1:B:371:ILE:HG23 | 1.64                     | 0.79              |
| 1:B:508:LEU:HD22 | 1:B:611:THR:HG21 | 1.65                     | 0.79              |
| 1:B:57:ILE:HG13  | 1:B:75:LYS:NZ    | 1.98                     | 0.79              |
| 1:B:653:VAL:HG13 | 1:B:692:ALA:HB3  | 1.64                     | 0.79              |
| 1:A:335:MSE:HE1  | 1:A:430:LYS:HG3  | 1.63                     | 0.78              |
| 1:C:219:LYS:HD3  | 1:C:358:HIS:H    | 1.48                     | 0.78              |
| 1:C:66:PRO:HD2   | 1:C:133:ASN:HD22 | 1.48                     | 0.78              |
| 1:E:24:ILE:HD11  | 1:E:56:PHE:HA    | 1.65                     | 0.78              |
| 1:E:282:ILE:HD12 | 1:E:371:ILE:HG23 | 1.65                     | 0.78              |
| 1:F:169:PRO:HG2  | 1:F:170:LEU:HD12 | 1.64                     | 0.78              |
| 1:D:219:LYS:HD3  | 1:D:358:HIS:H    | 1.49                     | 0.78              |
| 1:E:506:ILE:HB   | 1:E:711:LEU:HD12 | 1.65                     | 0.78              |
| 1:E:15:VAL:HG11  | 1:E:67:LEU:HB2   | 1.65                     | 0.78              |
| 1:F:249:PRO:HG3  | 1:F:300:LEU:HD13 | 1.65                     | 0.78              |
| 1:A:435:GLU:HA   | 1:A:438:ARG:HD2  | 1.63                     | 0.78              |
| 1:A:225:HIS:HA   | 1:A:330:ALA:HB2  | 1.66                     | 0.78              |
| 1:A:331:ASN:HD22 | 1:A:337:MSE:HA   | 1.48                     | 0.78              |
| 1:E:580:LYS:HG3  | 1:E:593:ASN:HD22 | 1.48                     | 0.78              |
| 1:B:14:ALA:HB3   | 1:B:103:PRO:CG   | 2.12                     | 0.78              |
| 1:C:690:ALA:HB1  | 1:C:725:ILE:HG13 | 1.66                     | 0.78              |
| 1:E:268:PRO:HG2  | 1:E:378:ARG:HH22 | 1.49                     | 0.78              |
| 1:F:269:GLU:HB2  | 1:F:378:ARG:CZ   | 2.14                     | 0.78              |
| 1:B:337:MSE:HE3  | 1:B:367:ASP:HA   | 1.65                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:494:VAL:HG22 | 1:C:738:VAL:HG22 | 1.66                     | 0.78              |
| 1:E:412:GLY:HA3  | 1:E:750:ASN:HD22 | 1.49                     | 0.78              |
| 1:A:267:SER:HB2  | 1:A:270:GLU:CB   | 2.14                     | 0.78              |
| 1:A:412:GLY:HA3  | 1:A:750:ASN:HD22 | 1.48                     | 0.78              |
| 1:B:526:TYR:O    | 1:B:532:VAL:HG13 | 1.83                     | 0.78              |
| 1:C:329:SER:HB2  | 1:C:331:ASN:HD21 | 1.49                     | 0.78              |
| 1:C:11:ILE:CG2   | 1:C:69:ARG:H     | 1.97                     | 0.78              |
| 1:E:368:ASP:HA   | 1:E:385:ARG:HD3  | 1.66                     | 0.78              |
| 1:E:30:LEU:HD13  | 1:E:52:ASP:HB2   | 1.65                     | 0.77              |
| 1:B:412:GLY:HA3  | 1:B:750:ASN:HD22 | 1.48                     | 0.77              |
| 1:D:553:PRO:HB2  | 1:D:620:VAL:HG21 | 1.64                     | 0.77              |
| 1:A:106:ILE:HG23 | 1:A:277:TYR:HB2  | 1.64                     | 0.77              |
| 1:A:183:VAL:HG23 | 1:A:184:CYS:N    | 1.99                     | 0.77              |
| 1:A:485:GLN:NE2  | 1:A:487:HIS:H    | 1.83                     | 0.77              |
| 1:D:380:VAL:HG23 | 1:D:740:THR:HA   | 1.66                     | 0.77              |
| 1:B:282:ILE:HG22 | 1:B:305:VAL:HB   | 1.65                     | 0.77              |
| 1:C:687:LEU:HB3  | 1:C:724:MSE:HE2  | 1.65                     | 0.77              |
| 1:D:88:ILE:HG22  | 1:D:89:GLU:N     | 1.99                     | 0.77              |
| 1:B:371:ILE:HD12 | 1:B:380:VAL:HG22 | 1.66                     | 0.77              |
| 1:C:207:ALA:O    | 1:C:210:ILE:HG22 | 1.85                     | 0.77              |
| 1:E:210:ILE:HD13 | 1:E:216:VAL:HG12 | 1.65                     | 0.77              |
| 1:F:6:ILE:HG23   | 1:F:73:ILE:HG23  | 1.67                     | 0.77              |
| 1:F:633:GLU:H    | 1:F:634:PRO:HD2  | 1.50                     | 0.76              |
| 1:C:456:ILE:HG22 | 1:C:457:ILE:H    | 1.50                     | 0.76              |
| 1:E:729:VAL:HG11 | 1:E:735:ASN:HB3  | 1.66                     | 0.76              |
| 1:F:373:PHE:CD1  | 1:F:378:ARG:HB3  | 2.21                     | 0.76              |
| 1:A:11:ILE:HG21  | 1:A:69:ARG:N     | 2.00                     | 0.76              |
| 1:B:165:GLU:HB3  | 1:B:171:ASN:ND2  | 2.01                     | 0.76              |
| 1:B:201:ASP:N    | 1:B:202:PRO:HD2  | 2.01                     | 0.76              |
| 1:C:690:ALA:HB2  | 1:C:721:ILE:HG23 | 1.68                     | 0.76              |
| 1:F:35:LYS:HG3   | 1:F:90:LYS:HD2   | 1.65                     | 0.76              |
| 1:B:267:SER:HB2  | 1:B:270:GLU:HB2  | 1.67                     | 0.76              |
| 1:B:494:VAL:HG11 | 1:B:710:ALA:HB1  | 1.68                     | 0.76              |
| 1:D:653:VAL:HG13 | 1:D:692:ALA:HB3  | 1.67                     | 0.76              |
| 1:A:236:VAL:HG13 | 1:A:295:ASN:HD22 | 1.50                     | 0.76              |
| 1:E:470:ALA:HB1  | 1:E:481:LEU:HD11 | 1.68                     | 0.76              |
| 1:C:287:LYS:HG3  | 1:C:289:PRO:HD2  | 1.68                     | 0.76              |
| 1:E:106:ILE:HG23 | 1:E:277:TYR:HB2  | 1.66                     | 0.76              |
| 1:A:371:ILE:HD12 | 1:A:380:VAL:HG22 | 1.68                     | 0.76              |
| 1:A:485:GLN:HG3  | 1:A:488:TYR:H    | 1.50                     | 0.76              |
| 1:D:601:LYS:HD3  | 1:E:772:LEU:HD11 | 1.68                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:128:PHE:HB3  | 1:B:360:ARG:NH2  | 2.01                     | 0.75              |
| 1:C:110:ASP:O    | 1:C:113:LEU:HB3  | 1.86                     | 0.75              |
| 1:C:11:ILE:HG21  | 1:C:69:ARG:H     | 1.49                     | 0.75              |
| 1:B:225:HIS:NE2  | 1:B:327:MSE:HE3  | 2.01                     | 0.75              |
| 1:E:329:SER:HB2  | 1:E:331:ASN:HD21 | 1.51                     | 0.75              |
| 1:E:371:ILE:HB   | 1:E:380:VAL:HG13 | 1.68                     | 0.75              |
| 1:F:404:GLY:HA2  | 1:F:753:GLN:NE2  | 2.00                     | 0.75              |
| 1:A:380:VAL:HG23 | 1:A:740:THR:HA   | 1.69                     | 0.75              |
| 1:C:198:ILE:HG13 | 1:D:122:LYS:CD   | 2.17                     | 0.75              |
| 1:E:165:GLU:HB3  | 1:E:171:ASN:ND2  | 2.01                     | 0.75              |
| 1:A:121:ASN:ND2  | 1:A:123:ARG:H    | 1.83                     | 0.75              |
| 1:B:557:LEU:HD12 | 1:B:620:VAL:HB   | 1.69                     | 0.75              |
| 1:D:589:LYS:HG3  | 1:D:590:VAL:H    | 1.51                     | 0.75              |
| 1:F:111:ASP:HB2  | 1:F:172:ARG:HH22 | 1.51                     | 0.75              |
| 1:F:255:LYS:HB2  | 1:F:323:PRO:HB3  | 1.69                     | 0.75              |
| 1:E:215:ILE:HG22 | 1:E:228:CYS:HB2  | 1.67                     | 0.75              |
| 1:A:190:LEU:O    | 1:A:196:GLN:HB2  | 1.87                     | 0.75              |
| 1:A:456:ILE:HG22 | 1:A:457:ILE:N    | 2.01                     | 0.75              |
| 1:A:628:ARG:HH21 | 1:A:632:GLY:H    | 1.33                     | 0.75              |
| 1:E:633:GLU:H    | 1:E:634:PRO:HD2  | 1.52                     | 0.75              |
| 1:A:502:SER:HB3  | 1:A:528:GLY:HA2  | 1.69                     | 0.74              |
| 1:A:765:LEU:HD21 | 1:A:770:LEU:HD21 | 1.69                     | 0.74              |
| 1:C:249:PRO:HG3  | 1:C:300:LEU:HD13 | 1.69                     | 0.74              |
| 1:B:52:ASP:O     | 1:B:56:PHE:HB2   | 1.87                     | 0.74              |
| 1:B:557:LEU:HD21 | 1:B:621:LEU:HD13 | 1.69                     | 0.74              |
| 1:D:169:PRO:HG2  | 1:D:170:LEU:HD12 | 1.67                     | 0.74              |
| 1:E:131:CYS:HB2  | 1:E:172:ARG:HG3  | 1.67                     | 0.74              |
| 1:F:15:VAL:HG12  | 1:F:16:GLY:H     | 1.51                     | 0.74              |
| 1:F:526:TYR:O    | 1:F:532:VAL:HG13 | 1.87                     | 0.74              |
| 1:B:456:ILE:HG22 | 1:B:457:ILE:N    | 2.02                     | 0.74              |
| 1:E:371:ILE:HD12 | 1:E:380:VAL:HG22 | 1.69                     | 0.74              |
| 1:B:427:ASN:ND2  | 1:B:429:GLY:H    | 1.84                     | 0.74              |
| 1:E:219:LYS:HG3  | 1:E:224:ILE:HG22 | 1.70                     | 0.74              |
| 1:B:633:GLU:H    | 1:B:634:PRO:HD2  | 1.52                     | 0.74              |
| 1:D:121:ASN:ND2  | 1:D:123:ARG:H    | 1.84                     | 0.74              |
| 1:E:508:LEU:HD22 | 1:E:611:THR:HG21 | 1.67                     | 0.74              |
| 1:B:287:LYS:HG3  | 1:B:289:PRO:HD2  | 1.68                     | 0.74              |
| 1:B:108:ILE:HD11 | 1:B:314:TYR:CD2  | 2.22                     | 0.74              |
| 1:D:371:ILE:HD12 | 1:D:380:VAL:HG22 | 1.70                     | 0.74              |
| 1:A:521:GLY:HA3  | 1:A:610:SER:HA   | 1.69                     | 0.74              |
| 1:B:208:GLU:O    | 1:B:212:LYS:HG2  | 1.87                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:270:GLU:OE1  | 1:E:284:LEU:HD21 | 1.87                     | 0.74              |
| 1:B:502:SER:HB3  | 1:B:528:GLY:HA2  | 1.68                     | 0.74              |
| 1:C:190:LEU:HB2  | 1:C:202:PRO:HB3  | 1.68                     | 0.74              |
| 1:C:273:GLU:HG2  | 1:C:371:ILE:HD13 | 1.69                     | 0.74              |
| 1:F:330:ALA:HB1  | 1:F:348:LEU:HD21 | 1.70                     | 0.74              |
| 1:B:35:LYS:HG2   | 1:B:36:ASN:H     | 1.53                     | 0.73              |
| 1:C:415:LYS:HD3  | 1:C:448:LEU:HD22 | 1.70                     | 0.73              |
| 1:E:539:ASP:HA   | 1:E:659:LEU:HD11 | 1.69                     | 0.73              |
| 1:A:461:HIS:CE1  | 1:A:463:ALA:HB3  | 2.23                     | 0.73              |
| 1:B:236:VAL:HG13 | 1:B:295:ASN:HD22 | 1.51                     | 0.73              |
| 1:C:373:PHE:CD1  | 1:C:378:ARG:HB3  | 2.24                     | 0.73              |
| 1:C:650:LYS:HD2  | 1:C:691:ARG:HH22 | 1.53                     | 0.73              |
| 1:D:35:LYS:HZ3   | 1:D:90:LYS:HD2   | 1.53                     | 0.73              |
| 1:E:144:LEU:HD12 | 1:E:447:ILE:HG23 | 1.69                     | 0.73              |
| 1:E:625:ALA:HB2  | 1:E:637:LYS:HD2  | 1.70                     | 0.73              |
| 1:F:215:ILE:HG22 | 1:F:228:CYS:HB2  | 1.69                     | 0.73              |
| 1:A:542:PRO:O    | 1:A:559:GLY:HA3  | 1.89                     | 0.73              |
| 1:B:181:CYS:SG   | 1:B:183:VAL:HG22 | 2.28                     | 0.73              |
| 1:F:201:ASP:N    | 1:F:202:PRO:HD2  | 2.02                     | 0.73              |
| 1:A:3:ALA:HB2    | 1:A:47:GLU:HA    | 1.70                     | 0.73              |
| 1:A:584:SER:HB3  | 1:A:589:LYS:HB3  | 1.70                     | 0.73              |
| 1:A:729:VAL:HG11 | 1:A:735:ASN:HB3  | 1.70                     | 0.73              |
| 1:B:485:GLN:HE21 | 1:B:487:HIS:N    | 1.84                     | 0.73              |
| 1:D:406:GLU:HG3  | 1:D:407:LEU:HG   | 1.69                     | 0.73              |
| 1:E:225:HIS:HA   | 1:E:330:ALA:HB2  | 1.71                     | 0.73              |
| 1:F:690:ALA:HB2  | 1:F:721:ILE:HG23 | 1.69                     | 0.73              |
| 1:B:550:SER:O    | 1:B:628:ARG:HG3  | 1.89                     | 0.73              |
| 1:E:691:ARG:HE   | 1:E:724:MSE:HE2  | 1.52                     | 0.73              |
| 1:B:225:HIS:HA   | 1:B:330:ALA:CB   | 2.18                     | 0.73              |
| 1:C:339:LYS:HG3  | 1:C:365:ARG:NH1  | 2.04                     | 0.73              |
| 1:D:219:LYS:HG3  | 1:D:224:ILE:HG22 | 1.69                     | 0.73              |
| 1:E:654:PRO:HG2  | 1:E:661:ARG:HB3  | 1.69                     | 0.73              |
| 1:A:111:ASP:HB3  | 1:A:172:ARG:HH12 | 1.52                     | 0.72              |
| 1:A:268:PRO:HG2  | 1:A:378:ARG:NH2  | 2.02                     | 0.72              |
| 1:C:292:LEU:HD13 | 1:C:293:PRO:HD2  | 1.71                     | 0.72              |
| 1:C:284:LEU:HD21 | 1:C:305:VAL:HG21 | 1.70                     | 0.72              |
| 1:C:11:ILE:O     | 1:C:11:ILE:HG13  | 1.88                     | 0.72              |
| 1:F:181:CYS:SG   | 1:F:183:VAL:HG22 | 2.28                     | 0.72              |
| 1:E:544:PRO:HG2  | 1:E:555:ARG:HB3  | 1.71                     | 0.72              |
| 1:C:589:LYS:H    | 1:F:475:ASN:ND2  | 1.86                     | 0.72              |
| 1:D:557:LEU:HD12 | 1:D:620:VAL:HB   | 1.71                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:3:ALA:HB2    | 1:E:47:GLU:HA    | 1.70                     | 0.72              |
| 1:C:30:LEU:HD13  | 1:C:52:ASP:HB2   | 1.70                     | 0.72              |
| 1:E:587:TYR:HD1  | 1:E:588:GLY:H    | 1.37                     | 0.72              |
| 1:C:485:GLN:NE2  | 1:C:514:GLY:HA2  | 2.05                     | 0.72              |
| 1:D:193:SER:O    | 1:D:194:ASP:HB2  | 1.89                     | 0.72              |
| 1:F:281:ILE:HG12 | 1:F:306:MSE:HG2  | 1.69                     | 0.72              |
| 1:B:254:ALA:HB1  | 1:B:259:THR:HB   | 1.69                     | 0.72              |
| 1:D:485:GLN:NE2  | 1:D:487:HIS:H    | 1.85                     | 0.72              |
| 1:B:169:PRO:HG2  | 1:B:170:LEU:HD12 | 1.71                     | 0.72              |
| 1:C:649:LEU:HB3  | 1:C:684:SER:HB3  | 1.70                     | 0.72              |
| 1:F:587:TYR:HD1  | 1:F:588:GLY:H    | 1.38                     | 0.72              |
| 1:A:15:VAL:HG12  | 1:A:16:GLY:H     | 1.55                     | 0.72              |
| 1:A:379:ALA:HB3  | 1:A:744:ARG:NH1  | 2.03                     | 0.72              |
| 1:D:225:HIS:NE2  | 1:D:327:MSE:HE3  | 2.04                     | 0.72              |
| 1:E:22:TYR:CD2   | 1:E:169:PRO:HB3  | 2.25                     | 0.72              |
| 1:E:239:LEU:O    | 1:E:243:THR:HG22 | 1.90                     | 0.72              |
| 1:E:404:GLY:HA2  | 1:E:753:GLN:HE22 | 1.53                     | 0.72              |
| 1:F:18:ARG:HB2   | 1:F:19:PRO:HD3   | 1.70                     | 0.72              |
| 1:F:191:TYR:HB2  | 1:F:355:PHE:HB2  | 1.71                     | 0.72              |
| 1:A:148:ARG:O    | 1:A:151:THR:HG22 | 1.89                     | 0.71              |
| 1:A:274:LEU:HB3  | 1:A:307:LEU:HD11 | 1.70                     | 0.71              |
| 1:C:369:SER:H    | 1:C:385:ARG:CB   | 2.03                     | 0.71              |
| 1:F:108:ILE:HA   | 1:F:134:CYS:SG   | 2.31                     | 0.71              |
| 1:F:331:ASN:HD22 | 1:F:337:MSE:HA   | 1.55                     | 0.71              |
| 1:D:210:ILE:HD13 | 1:D:216:VAL:HG12 | 1.73                     | 0.71              |
| 1:F:726:ARG:NH2  | 1:F:727:LYS:HG2  | 2.05                     | 0.71              |
| 1:A:225:HIS:NE2  | 1:A:327:MSE:HE3  | 2.05                     | 0.71              |
| 1:D:201:ASP:N    | 1:D:202:PRO:HD2  | 2.05                     | 0.71              |
| 1:F:373:PHE:CE1  | 1:F:378:ARG:HB3  | 2.25                     | 0.71              |
| 1:F:491:ILE:HG23 | 1:F:507:ALA:HB2  | 1.71                     | 0.71              |
| 1:B:371:ILE:HB   | 1:B:380:VAL:HG13 | 1.72                     | 0.71              |
| 1:B:373:PHE:CE1  | 1:B:378:ARG:HB3  | 2.26                     | 0.71              |
| 1:B:380:VAL:HG12 | 1:B:381:ILE:H    | 1.56                     | 0.71              |
| 1:E:153:MSE:CE   | 1:E:360:ARG:HD2  | 2.20                     | 0.71              |
| 1:A:258:GLU:HA   | 1:A:261:LYS:HD3  | 1.73                     | 0.71              |
| 1:B:20:PHE:CZ    | 1:B:63:LYS:HB2   | 2.25                     | 0.71              |
| 1:D:11:ILE:HG21  | 1:D:69:ARG:H     | 1.56                     | 0.71              |
| 1:E:724:MSE:O    | 1:E:728:VAL:HG23 | 1.91                     | 0.71              |
| 1:D:170:LEU:HD12 | 1:D:170:LEU:H    | 1.54                     | 0.71              |
| 1:D:330:ALA:HB1  | 1:D:348:LEU:HD21 | 1.71                     | 0.71              |
| 1:D:539:ASP:HA   | 1:D:659:LEU:HD11 | 1.72                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:108:ILE:HA   | 1:B:134:CYS:SG   | 2.31                     | 0.71              |
| 1:C:149:GLU:HA   | 1:C:154:LYS:HG2  | 1.72                     | 0.71              |
| 1:D:274:LEU:HD22 | 1:D:307:LEU:HG   | 1.72                     | 0.71              |
| 1:E:207:ALA:O    | 1:E:210:ILE:HG22 | 1.89                     | 0.71              |
| 1:E:633:GLU:N    | 1:E:634:PRO:HD2  | 2.04                     | 0.71              |
| 1:F:543:LEU:HD12 | 1:F:549:ALA:HB3  | 1.73                     | 0.71              |
| 1:B:279:ARG:HD3  | 1:B:307:LEU:HB2  | 1.72                     | 0.71              |
| 1:C:404:GLY:HA2  | 1:C:753:GLN:NE2  | 2.06                     | 0.71              |
| 1:D:225:HIS:HA   | 1:D:330:ALA:CB   | 2.20                     | 0.71              |
| 1:F:554:LEU:O    | 1:F:558:MSE:HG3  | 1.89                     | 0.71              |
| 1:B:495:MSE:HE2  | 1:B:755:PHE:HZ   | 1.55                     | 0.70              |
| 1:C:136:PRO:HG3  | 1:C:360:ARG:NH1  | 2.06                     | 0.70              |
| 1:D:142:GLU:HB3  | 1:D:150:ASN:O    | 1.91                     | 0.70              |
| 1:D:485:GLN:HG3  | 1:D:488:TYR:H    | 1.55                     | 0.70              |
| 1:E:445:ARG:HH21 | 1:E:452:ASN:HD22 | 1.39                     | 0.70              |
| 1:E:583:GLU:CD   | 1:E:583:GLU:H    | 1.95                     | 0.70              |
| 1:E:553:PRO:HB2  | 1:E:620:VAL:HG21 | 1.73                     | 0.70              |
| 1:F:687:LEU:HD22 | 1:F:724:MSE:HB2  | 1.72                     | 0.70              |
| 1:F:6:ILE:HG22   | 1:F:7:HIS:H      | 1.56                     | 0.70              |
| 1:A:26:HIS:HE1   | 1:A:87:TYR:HB3   | 1.57                     | 0.70              |
| 1:F:413:VAL:HG21 | 1:F:448:LEU:HD13 | 1.73                     | 0.70              |
| 1:A:526:TYR:O    | 1:A:532:VAL:HG13 | 1.91                     | 0.70              |
| 1:F:144:LEU:HD12 | 1:F:447:ILE:HG23 | 1.73                     | 0.70              |
| 1:F:89:GLU:HG3   | 1:F:175:HIS:HE2  | 1.56                     | 0.70              |
| 1:B:590:VAL:O    | 1:B:594:VAL:HG23 | 1.92                     | 0.70              |
| 1:E:495:MSE:HE2  | 1:E:755:PHE:HZ   | 1.56                     | 0.70              |
| 1:F:391:PRO:HB2  | 1:F:418:LYS:HB2  | 1.72                     | 0.70              |
| 1:B:18:ARG:HB2   | 1:B:19:PRO:HD3   | 1.74                     | 0.70              |
| 1:A:601:LYS:HD3  | 1:B:772:LEU:HD11 | 1.74                     | 0.70              |
| 1:C:391:PRO:HB3  | 1:C:420:TYR:CE1  | 2.27                     | 0.70              |
| 1:D:144:LEU:HD12 | 1:D:447:ILE:HG23 | 1.74                     | 0.70              |
| 1:D:694:ALA:HB2  | 1:D:725:ILE:HG23 | 1.74                     | 0.70              |
| 1:A:207:ALA:HB1  | 1:A:320:SER:HB2  | 1.73                     | 0.70              |
| 1:B:567:ILE:HG12 | 1:B:600:ALA:HB1  | 1.74                     | 0.70              |
| 1:D:190:LEU:HB2  | 1:D:202:PRO:HB2  | 1.72                     | 0.70              |
| 1:D:13:GLN:HE21  | 1:D:42:VAL:HG23  | 1.56                     | 0.70              |
| 1:D:6:ILE:HB     | 1:D:44:ILE:HB    | 1.73                     | 0.70              |
| 1:D:8:VAL:HA     | 1:D:72:ARG:HB2   | 1.74                     | 0.70              |
| 1:F:14:ALA:HB3   | 1:F:103:PRO:HD3  | 1.73                     | 0.70              |
| 1:B:144:LEU:HD12 | 1:B:447:ILE:HG23 | 1.73                     | 0.70              |
| 1:A:516:ASP:HA   | 1:B:603:ILE:HG23 | 1.73                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:18:ARG:HB2   | 1:C:19:PRO:HD3   | 1.74                     | 0.70              |
| 1:D:329:SER:HB2  | 1:D:331:ASN:HD21 | 1.56                     | 0.70              |
| 1:E:14:ALA:O     | 1:E:103:PRO:HG3  | 1.92                     | 0.70              |
| 1:E:292:LEU:HD11 | 1:E:324:VAL:HG21 | 1.74                     | 0.70              |
| 1:E:330:ALA:HB1  | 1:E:348:LEU:HD21 | 1.74                     | 0.70              |
| 1:F:434:LEU:HD13 | 1:F:465:ASN:HB3  | 1.72                     | 0.70              |
| 1:D:263:PHE:HZ   | 1:D:303:ILE:HG21 | 1.56                     | 0.70              |
| 1:F:225:HIS:NE2  | 1:F:327:MSE:HE3  | 2.07                     | 0.70              |
| 1:E:208:GLU:O    | 1:E:212:LYS:HG2  | 1.91                     | 0.69              |
| 1:F:409:ASN:HD22 | 1:F:425:ILE:HD11 | 1.56                     | 0.69              |
| 1:C:506:ILE:HD11 | 1:C:694:ALA:HA   | 1.74                     | 0.69              |
| 1:A:504:ILE:O    | 1:A:709:VAL:HA   | 1.91                     | 0.69              |
| 1:A:649:LEU:HD12 | 1:A:650:LYS:H    | 1.56                     | 0.69              |
| 1:D:207:ALA:O    | 1:D:210:ILE:HG22 | 1.91                     | 0.69              |
| 1:D:374:VAL:HG21 | 1:D:744:ARG:NH2  | 2.07                     | 0.69              |
| 1:F:127:PRO:O    | 1:F:311:GLY:HA3  | 1.92                     | 0.69              |
| 1:A:379:ALA:CB   | 1:A:744:ARG:HH11 | 2.04                     | 0.69              |
| 1:B:215:ILE:HD11 | 1:B:352:ALA:HA   | 1.72                     | 0.69              |
| 1:C:281:ILE:HG12 | 1:C:306:MSE:HG3  | 1.74                     | 0.69              |
| 1:F:495:MSE:HE2  | 1:F:755:PHE:HZ   | 1.57                     | 0.69              |
| 1:A:207:ALA:O    | 1:A:210:ILE:HG22 | 1.92                     | 0.69              |
| 1:A:380:VAL:HG12 | 1:A:381:ILE:N    | 2.06                     | 0.69              |
| 1:B:20:PHE:HZ    | 1:B:63:LYS:HB2   | 1.57                     | 0.69              |
| 1:D:205:LYS:O    | 1:D:209:LEU:HD13 | 1.92                     | 0.69              |
| 1:D:287:LYS:HG3  | 1:D:289:PRO:HD2  | 1.74                     | 0.69              |
| 1:D:582:VAL:HG11 | 1:D:626:TYR:O    | 1.92                     | 0.69              |
| 1:E:190:LEU:HB2  | 1:E:202:PRO:HB3  | 1.74                     | 0.69              |
| 1:F:210:ILE:HD11 | 1:F:227:ALA:C    | 2.12                     | 0.69              |
| 1:A:227:ALA:HA   | 1:A:326:VAL:O    | 1.92                     | 0.69              |
| 1:A:32:GLY:O     | 1:A:87:TYR:HA    | 1.93                     | 0.69              |
| 1:A:472:GLU:O    | 1:A:476:GLU:HG2  | 1.92                     | 0.69              |
| 1:B:589:LYS:HG3  | 1:B:590:VAL:H    | 1.58                     | 0.69              |
| 1:C:317:PHE:HE2  | 1:C:323:PRO:HA   | 1.57                     | 0.69              |
| 1:A:329:SER:HA   | 1:A:337:MSE:HE2  | 1.73                     | 0.69              |
| 1:A:339:LYS:HA   | 1:A:362:ILE:HD11 | 1.74                     | 0.69              |
| 1:B:729:VAL:HB   | 1:B:735:ASN:HD22 | 1.57                     | 0.69              |
| 1:D:409:ASN:HD22 | 1:D:425:ILE:HD11 | 1.57                     | 0.69              |
| 1:B:207:ALA:O    | 1:B:210:ILE:HG22 | 1.92                     | 0.69              |
| 1:C:329:SER:HB2  | 1:C:331:ASN:ND2  | 2.08                     | 0.69              |
| 1:D:633:GLU:H    | 1:D:634:PRO:HD2  | 1.57                     | 0.69              |
| 1:E:193:SER:O    | 1:E:194:ASP:HB2  | 1.93                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:282:ILE:HG22 | 1:E:305:VAL:HB   | 1.75                     | 0.69              |
| 1:A:662:VAL:O    | 1:A:665:LEU:HB3  | 1.93                     | 0.69              |
| 1:B:13:GLN:NE2   | 1:B:18:ARG:HH21  | 1.90                     | 0.69              |
| 1:B:752:GLY:O    | 1:B:756:LEU:HB2  | 1.92                     | 0.69              |
| 1:C:435:GLU:HA   | 1:C:438:ARG:HD2  | 1.74                     | 0.69              |
| 1:C:57:ILE:HG21  | 1:C:75:LYS:HE3   | 1.74                     | 0.69              |
| 1:D:315:ILE:HG12 | 1:D:319:TRP:HZ3  | 1.56                     | 0.69              |
| 1:F:19:PRO:HA    | 1:F:174:TYR:CD1  | 2.28                     | 0.69              |
| 1:F:537:HIS:NE2  | 1:F:659:LEU:HD22 | 2.07                     | 0.69              |
| 1:A:383:ARG:HH21 | 1:A:392:ILE:HD11 | 1.57                     | 0.68              |
| 1:E:267:SER:O    | 1:E:270:GLU:HB3  | 1.91                     | 0.68              |
| 1:A:689:LEU:O    | 1:A:693:PHE:HB2  | 1.93                     | 0.68              |
| 1:A:590:VAL:H    | 1:B:475:ASN:HD21 | 1.41                     | 0.68              |
| 1:C:385:ARG:HG3  | 1:C:386:GLY:H    | 1.58                     | 0.68              |
| 1:E:572:GLY:HA2  | 1:E:575:ASN:HD22 | 1.57                     | 0.68              |
| 1:F:288:GLU:CB   | 1:F:289:PRO:HD3  | 2.22                     | 0.68              |
| 1:F:760:TYR:HE2  | 1:F:767:LYS:HG2  | 1.59                     | 0.68              |
| 1:B:369:SER:HB2  | 1:B:385:ARG:CB   | 2.24                     | 0.68              |
| 1:C:26:HIS:CE1   | 1:C:87:TYR:HB3   | 2.28                     | 0.68              |
| 1:D:391:PRO:HB3  | 1:D:420:TYR:CE1  | 2.29                     | 0.68              |
| 1:F:267:SER:HB2  | 1:F:270:GLU:HB2  | 1.76                     | 0.68              |
| 1:E:6:ILE:HA     | 1:E:74:GLU:O     | 1.93                     | 0.68              |
| 1:A:215:ILE:HG22 | 1:A:228:CYS:HB2  | 1.74                     | 0.68              |
| 1:B:514:GLY:HA3  | 1:B:520:TRP:CD1  | 2.29                     | 0.68              |
| 1:D:369:SER:H    | 1:D:385:ARG:CB   | 2.06                     | 0.68              |
| 1:E:639:GLU:HB2  | 1:E:718:ASN:HD21 | 1.58                     | 0.68              |
| 1:F:230:ALA:HB3  | 1:F:324:VAL:HB   | 1.75                     | 0.68              |
| 1:A:247:GLN:HE22 | 1:A:637:LYS:HE3  | 1.59                     | 0.68              |
| 1:B:534:ARG:HG2  | 1:B:535:LEU:N    | 2.08                     | 0.68              |
| 1:C:355:PHE:HB3  | 1:C:357:LEU:HD21 | 1.75                     | 0.68              |
| 1:C:61:TYR:OH    | 1:C:73:ILE:HG21  | 1.92                     | 0.68              |
| 1:C:88:ILE:HG22  | 1:C:89:GLU:H     | 1.57                     | 0.68              |
| 1:E:229:ASP:OD1  | 1:E:322:THR:HG21 | 1.94                     | 0.68              |
| 1:F:394:ILE:CD1  | 1:F:419:VAL:HB   | 2.21                     | 0.68              |
| 1:D:373:PHE:CD1  | 1:D:378:ARG:HB3  | 2.28                     | 0.68              |
| 1:E:8:VAL:HB     | 1:E:42:VAL:HB    | 1.75                     | 0.68              |
| 1:F:208:GLU:O    | 1:F:212:LYS:HG2  | 1.94                     | 0.68              |
| 1:F:653:VAL:HG11 | 1:F:689:LEU:HA   | 1.76                     | 0.68              |
| 1:F:649:LEU:HB3  | 1:F:684:SER:HB3  | 1.76                     | 0.68              |
| 1:A:553:PRO:CB   | 1:A:620:VAL:HG21 | 2.24                     | 0.68              |
| 1:A:687:LEU:HD22 | 1:A:724:MSE:HE3  | 1.74                     | 0.68              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:460:LEU:O    | 1:C:462:PRO:HD3  | 1.94                     | 0.68              |
| 1:F:341:ASN:HD22 | 1:F:357:LEU:HB3  | 1.59                     | 0.68              |
| 1:B:286:LYS:HD2  | 1:B:303:ILE:HD11 | 1.75                     | 0.67              |
| 1:B:469:LEU:HG   | 1:B:473:MSE:HG3  | 1.75                     | 0.67              |
| 1:B:460:LEU:HD12 | 1:B:483:GLN:HB3  | 1.76                     | 0.67              |
| 1:B:524:VAL:HG22 | 1:B:536:ALA:HB3  | 1.76                     | 0.67              |
| 1:C:589:LYS:HG3  | 1:C:590:VAL:H    | 1.57                     | 0.67              |
| 1:F:165:GLU:HB3  | 1:F:171:ASN:ND2  | 2.09                     | 0.67              |
| 1:A:15:VAL:HG11  | 1:A:67:LEU:O     | 1.94                     | 0.67              |
| 1:A:419:VAL:HG11 | 1:A:751:VAL:HG23 | 1.76                     | 0.67              |
| 1:D:12:VAL:HG13  | 1:D:17:PHE:CG    | 2.29                     | 0.67              |
| 1:D:219:LYS:HE3  | 1:D:358:HIS:CE1  | 2.29                     | 0.67              |
| 1:D:504:ILE:HG22 | 1:D:505:GLY:N    | 2.10                     | 0.67              |
| 1:E:282:ILE:HG13 | 1:E:283:THR:H    | 1.60                     | 0.67              |
| 1:F:12:VAL:HG13  | 1:F:42:VAL:HG21  | 1.76                     | 0.67              |
| 1:F:503:VAL:HB   | 1:F:708:ASN:O    | 1.94                     | 0.67              |
| 1:A:249:PRO:HG3  | 1:A:300:LEU:HD13 | 1.76                     | 0.67              |
| 1:A:373:PHE:CD1  | 1:A:378:ARG:HB3  | 2.29                     | 0.67              |
| 1:B:624:VAL:O    | 1:B:625:ALA:HB2  | 1.93                     | 0.67              |
| 1:C:267:SER:O    | 1:C:270:GLU:HB3  | 1.93                     | 0.67              |
| 1:D:32:GLY:O     | 1:D:87:TYR:HA    | 1.94                     | 0.67              |
| 1:E:408:MSE:HG3  | 1:E:424:TYR:CE1  | 2.29                     | 0.67              |
| 1:A:102:ILE:HD11 | 1:A:144:LEU:HG   | 1.77                     | 0.67              |
| 1:C:131:CYS:HB2  | 1:C:172:ARG:HG3  | 1.76                     | 0.67              |
| 1:C:30:LEU:HG    | 1:C:47:GLU:O     | 1.94                     | 0.67              |
| 1:E:121:ASN:ND2  | 1:E:123:ARG:H    | 1.92                     | 0.67              |
| 1:E:428:THR:HA   | 1:E:433:VAL:HG11 | 1.76                     | 0.67              |
| 1:F:544:PRO:HG2  | 1:F:555:ARG:HB3  | 1.76                     | 0.67              |
| 1:C:369:SER:N    | 1:C:385:ARG:HB2  | 2.10                     | 0.67              |
| 1:D:491:ILE:HD11 | 1:D:505:GLY:HA3  | 1.75                     | 0.67              |
| 1:A:391:PRO:HB3  | 1:A:420:TYR:CE1  | 2.29                     | 0.67              |
| 1:A:6:ILE:HD12   | 1:A:73:ILE:HG23  | 1.76                     | 0.67              |
| 1:C:148:ARG:O    | 1:C:151:THR:HG22 | 1.94                     | 0.67              |
| 1:E:183:VAL:HG23 | 1:E:184:CYS:N    | 2.09                     | 0.67              |
| 1:F:620:VAL:HG13 | 1:F:626:TYR:CD1  | 2.29                     | 0.67              |
| 1:A:544:PRO:HD2  | 1:A:555:ARG:O    | 1.94                     | 0.67              |
| 1:C:253:MSE:HE3  | 1:C:308:PRO:HB3  | 1.77                     | 0.67              |
| 1:D:369:SER:HB2  | 1:D:385:ARG:HB3  | 1.75                     | 0.67              |
| 1:F:168:ASP:O    | 1:F:174:TYR:HB2  | 1.95                     | 0.67              |
| 1:A:219:LYS:HA   | 1:A:224:ILE:HG22 | 1.76                     | 0.67              |
| 1:B:394:ILE:HG23 | 1:B:755:PHE:HB2  | 1.76                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:503:VAL:HB   | 1:B:708:ASN:O    | 1.94                     | 0.67              |
| 1:C:170:LEU:H    | 1:C:170:LEU:HD12 | 1.60                     | 0.67              |
| 1:C:13:GLN:HE21  | 1:C:42:VAL:HG23  | 1.58                     | 0.67              |
| 1:C:521:GLY:HA3  | 1:C:610:SER:HA   | 1.76                     | 0.67              |
| 1:E:415:LYS:HD3  | 1:E:448:LEU:HD22 | 1.77                     | 0.67              |
| 1:A:225:HIS:HA   | 1:A:330:ALA:CB   | 2.24                     | 0.67              |
| 1:C:102:ILE:HG23 | 1:C:141:ILE:HD13 | 1.76                     | 0.67              |
| 1:D:526:TYR:O    | 1:D:532:VAL:HG13 | 1.95                     | 0.67              |
| 1:A:148:ARG:NH2  | 1:A:158:MSE:HG3  | 2.08                     | 0.67              |
| 1:B:288:GLU:CB   | 1:B:289:PRO:HD3  | 2.23                     | 0.67              |
| 1:E:394:ILE:HG23 | 1:E:755:PHE:HB2  | 1.76                     | 0.67              |
| 1:F:250:PHE:HE2  | 1:F:328:THR:HG1  | 1.43                     | 0.67              |
| 1:B:268:PRO:HG2  | 1:B:378:ARG:NH2  | 2.07                     | 0.66              |
| 1:D:163:ARG:HB2  | 1:D:163:ARG:HH11 | 1.60                     | 0.66              |
| 1:D:191:TYR:HB2  | 1:D:355:PHE:HB2  | 1.77                     | 0.66              |
| 1:D:554:LEU:O    | 1:D:558:MSE:HG3  | 1.96                     | 0.66              |
| 1:E:738:VAL:HG12 | 1:E:742:VAL:HB   | 1.76                     | 0.66              |
| 1:F:396:PHE:CZ   | 1:F:759:LEU:HD13 | 2.30                     | 0.66              |
| 1:C:34:VAL:HB    | 1:C:87:TYR:OH    | 1.95                     | 0.66              |
| 1:C:508:LEU:HD22 | 1:C:611:THR:HG21 | 1.77                     | 0.66              |
| 1:C:649:LEU:HB3  | 1:C:684:SER:CB   | 2.25                     | 0.66              |
| 1:D:269:GLU:HB2  | 1:D:378:ARG:CZ   | 2.25                     | 0.66              |
| 1:A:261:LYS:HG3  | 1:A:266:VAL:HG21 | 1.75                     | 0.66              |
| 1:A:616:ASP:OD2  | 1:A:634:PRO:HG3  | 1.94                     | 0.66              |
| 1:C:738:VAL:HG12 | 1:C:742:VAL:O    | 1.95                     | 0.66              |
| 1:D:279:ARG:HD2  | 1:D:308:PRO:O    | 1.96                     | 0.66              |
| 1:E:373:PHE:CD1  | 1:E:378:ARG:HB3  | 2.30                     | 0.66              |
| 1:F:398:TYR:HB2  | 1:F:454:ASP:OD2  | 1.95                     | 0.66              |
| 1:F:580:LYS:HZ2  | 1:F:590:VAL:HG13 | 1.60                     | 0.66              |
| 1:C:461:HIS:CE1  | 1:C:463:ALA:HB3  | 2.31                     | 0.66              |
| 1:F:89:GLU:HG3   | 1:F:175:HIS:NE2  | 2.10                     | 0.66              |
| 1:B:156:PHE:HZ   | 1:B:359:ASN:HB2  | 1.61                     | 0.66              |
| 1:B:394:ILE:HG22 | 1:B:396:PHE:H    | 1.59                     | 0.66              |
| 1:F:264:ALA:CB   | 1:F:286:LYS:HA   | 2.25                     | 0.66              |
| 1:F:412:GLY:HA3  | 1:F:750:ASN:ND2  | 2.11                     | 0.66              |
| 1:B:267:SER:HB2  | 1:B:270:GLU:CB   | 2.26                     | 0.66              |
| 1:D:215:ILE:HG22 | 1:D:228:CYS:HB2  | 1.78                     | 0.66              |
| 1:D:508:LEU:HD22 | 1:D:611:THR:HG21 | 1.78                     | 0.66              |
| 1:E:504:ILE:HB   | 1:E:709:VAL:HG12 | 1.77                     | 0.66              |
| 1:F:203:LEU:HD12 | 1:F:319:TRP:HZ3  | 1.61                     | 0.66              |
| 1:B:142:GLU:HG3  | 1:B:143:ASP:OD1  | 1.95                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:227:ALA:HA   | 1:B:326:VAL:O    | 1.96                     | 0.66              |
| 1:D:137:ARG:NH2  | 1:D:178:PRO:HG3  | 2.10                     | 0.66              |
| 1:E:267:SER:HB2  | 1:E:270:GLU:HB2  | 1.77                     | 0.66              |
| 1:F:261:LYS:HZ1  | 1:F:266:VAL:HB   | 1.61                     | 0.66              |
| 1:B:22:TYR:CD2   | 1:B:169:PRO:HB3  | 2.31                     | 0.66              |
| 1:C:756:LEU:O    | 1:C:759:LEU:HB3  | 1.96                     | 0.66              |
| 1:D:580:LYS:HG3  | 1:D:593:ASN:HD22 | 1.61                     | 0.66              |
| 1:E:286:LYS:HD2  | 1:E:303:ILE:HD11 | 1.78                     | 0.66              |
| 1:A:589:LYS:HG3  | 1:A:590:VAL:N    | 2.11                     | 0.66              |
| 1:C:506:ILE:HG12 | 1:C:524:VAL:HG12 | 1.78                     | 0.66              |
| 1:C:484:VAL:HG12 | 1:C:770:LEU:HD22 | 1.77                     | 0.66              |
| 1:D:384:SER:HA   | 1:D:388:VAL:HG23 | 1.78                     | 0.66              |
| 1:D:502:SER:HB3  | 1:D:528:GLY:HA2  | 1.77                     | 0.66              |
| 1:E:312:THR:HA   | 1:E:315:ILE:HG22 | 1.78                     | 0.66              |
| 1:A:425:ILE:HA   | 1:A:436:PHE:HE1  | 1.59                     | 0.66              |
| 1:C:200:GLY:C    | 1:C:202:PRO:HD2  | 2.16                     | 0.66              |
| 1:C:337:MSE:HG3  | 1:C:367:ASP:OD2  | 1.96                     | 0.66              |
| 1:C:698:VAL:HG13 | 1:C:732:ASN:HD22 | 1.61                     | 0.66              |
| 1:D:239:LEU:O    | 1:D:243:THR:HG22 | 1.96                     | 0.66              |
| 1:E:649:LEU:HB3  | 1:E:684:SER:HB3  | 1.78                     | 0.66              |
| 1:C:103:PRO:CG   | 1:C:137:ARG:HD2  | 2.25                     | 0.65              |
| 1:C:66:PRO:CD    | 1:C:133:ASN:HD22 | 2.08                     | 0.65              |
| 1:D:491:ILE:HG23 | 1:D:527:LEU:HD21 | 1.76                     | 0.65              |
| 1:E:263:PHE:HZ   | 1:E:303:ILE:HG21 | 1.61                     | 0.65              |
| 1:F:301:HIS:HD2  | 1:F:302:THR:H    | 1.44                     | 0.65              |
| 1:A:485:GLN:HE21 | 1:A:487:HIS:N    | 1.90                     | 0.65              |
| 1:A:490:HIS:HE1  | 1:A:746:ASP:HA   | 1.61                     | 0.65              |
| 1:C:412:GLY:HA3  | 1:C:750:ASN:HD22 | 1.61                     | 0.65              |
| 1:D:9:GLN:NE2    | 1:D:41:GLY:HA2   | 2.02                     | 0.65              |
| 1:D:700:ARG:HH11 | 1:D:704:PHE:HE2  | 1.43                     | 0.65              |
| 1:F:239:LEU:HD22 | 1:F:250:PHE:HZ   | 1.62                     | 0.65              |
| 1:C:591:GLU:HG2  | 1:F:475:ASN:HD22 | 1.61                     | 0.65              |
| 1:F:570:LEU:O    | 1:F:573:VAL:HG12 | 1.97                     | 0.65              |
| 1:F:649:LEU:HD12 | 1:F:650:LYS:H    | 1.61                     | 0.65              |
| 1:D:570:LEU:O    | 1:D:573:VAL:HG12 | 1.97                     | 0.65              |
| 1:F:615:LEU:CD1  | 1:F:638:LEU:HD23 | 2.25                     | 0.65              |
| 1:F:619:ALA:HB1  | 1:F:625:ALA:HB3  | 1.76                     | 0.65              |
| 1:A:166:TYR:CE1  | 1:A:175:HIS:HA   | 2.31                     | 0.65              |
| 1:A:508:LEU:HD22 | 1:A:611:THR:HG21 | 1.79                     | 0.65              |
| 1:C:743:PRO:HG2  | 1:C:748:GLY:HA3  | 1.79                     | 0.65              |
| 1:D:181:CYS:SG   | 1:D:183:VAL:HG13 | 2.37                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:12:VAL:HG23  | 1:E:68:ALA:HB1   | 1.79                     | 0.65              |
| 1:B:425:ILE:HG22 | 1:B:436:PHE:HE1  | 1.61                     | 0.65              |
| 1:B:456:ILE:HD12 | 1:B:480:GLU:O    | 1.97                     | 0.65              |
| 1:C:376:GLY:O    | 1:C:377:LYS:HG3  | 1.95                     | 0.65              |
| 1:E:270:GLU:OE2  | 1:E:284:LEU:HD11 | 1.97                     | 0.65              |
| 1:E:404:GLY:HA2  | 1:E:753:GLN:NE2  | 2.10                     | 0.65              |
| 1:F:409:ASN:HB3  | 1:F:425:ILE:HD11 | 1.78                     | 0.65              |
| 1:F:616:ASP:OD1  | 1:F:634:PRO:HG2  | 1.97                     | 0.65              |
| 1:F:641:PHE:HZ   | 1:F:678:PRO:HB2  | 1.61                     | 0.65              |
| 1:C:620:VAL:HG22 | 1:C:626:TYR:HA   | 1.79                     | 0.65              |
| 1:E:12:VAL:HA    | 1:E:68:ALA:HB1   | 1.77                     | 0.65              |
| 1:A:317:PHE:HE2  | 1:A:323:PRO:HA   | 1.62                     | 0.65              |
| 1:C:522:GLY:HA3  | 1:C:538:ILE:HD12 | 1.79                     | 0.65              |
| 1:D:155:GLU:O    | 1:D:157:PRO:HD3  | 1.96                     | 0.65              |
| 1:D:20:PHE:HA    | 1:D:23:ARG:HH21  | 1.60                     | 0.65              |
| 1:F:504:ILE:HG22 | 1:F:505:GLY:N    | 2.11                     | 0.65              |
| 1:A:337:MSE:HG3  | 1:A:367:ASP:OD2  | 1.97                     | 0.65              |
| 1:B:279:ARG:HB2  | 1:B:309:TYR:HB3  | 1.79                     | 0.65              |
| 1:B:481:LEU:HD12 | 1:B:482:LEU:H    | 1.62                     | 0.65              |
| 1:C:127:PRO:O    | 1:C:311:GLY:HA3  | 1.96                     | 0.65              |
| 1:D:233:GLU:HB2  | 1:D:295:ASN:ND2  | 2.11                     | 0.65              |
| 1:F:456:ILE:HG22 | 1:F:457:ILE:N    | 2.12                     | 0.65              |
| 1:A:165:GLU:HB3  | 1:A:171:ASN:ND2  | 2.11                     | 0.65              |
| 1:C:371:ILE:HB   | 1:C:380:VAL:HG13 | 1.78                     | 0.65              |
| 1:D:456:ILE:HG22 | 1:D:457:ILE:H    | 1.60                     | 0.65              |
| 1:E:590:VAL:O    | 1:E:594:VAL:HG23 | 1.96                     | 0.65              |
| 1:F:408:MSE:HG3  | 1:F:424:TYR:CE1  | 2.32                     | 0.65              |
| 1:F:694:ALA:HB2  | 1:F:725:ILE:HG12 | 1.79                     | 0.65              |
| 1:B:690:ALA:HB1  | 1:B:725:ILE:HG13 | 1.79                     | 0.65              |
| 1:B:498:LYS:HE3  | 1:B:736:PHE:HB2  | 1.79                     | 0.65              |
| 1:C:700:ARG:HH11 | 1:C:704:PHE:HE2  | 1.43                     | 0.65              |
| 1:E:232:ASN:HB3  | 1:E:235:VAL:HG22 | 1.79                     | 0.65              |
| 1:E:30:LEU:CD1   | 1:E:52:ASP:HB2   | 2.27                     | 0.65              |
| 1:F:743:PRO:HG2  | 1:F:748:GLY:HA3  | 1.79                     | 0.65              |
| 1:A:26:HIS:CE1   | 1:A:87:TYR:HB3   | 2.31                     | 0.64              |
| 1:A:619:ALA:O    | 1:A:624:VAL:HB   | 1.97                     | 0.64              |
| 1:B:215:ILE:O    | 1:B:353:ASP:HB2  | 1.97                     | 0.64              |
| 1:A:589:LYS:H    | 1:B:475:ASN:ND2  | 1.95                     | 0.64              |
| 1:B:374:VAL:HG21 | 1:B:744:ARG:NH2  | 2.12                     | 0.64              |
| 1:C:281:ILE:HG12 | 1:C:306:MSE:CG   | 2.27                     | 0.64              |
| 1:C:385:ARG:HG3  | 1:C:386:GLY:N    | 2.12                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:649:LEU:HD12 | 1:E:650:LYS:H    | 1.60                     | 0.64              |
| 1:B:263:PHE:HZ   | 1:B:303:ILE:HG21 | 1.62                     | 0.64              |
| 1:D:690:ALA:HB1  | 1:D:725:ILE:HG13 | 1.79                     | 0.64              |
| 1:E:103:PRO:HG2  | 1:E:137:ARG:HD2  | 1.78                     | 0.64              |
| 1:E:137:ARG:O    | 1:E:141:ILE:HG13 | 1.97                     | 0.64              |
| 1:E:281:ILE:HG12 | 1:E:306:MSE:CG   | 2.27                     | 0.64              |
| 1:E:329:SER:HA   | 1:E:337:MSE:HE2  | 1.80                     | 0.64              |
| 1:E:570:LEU:O    | 1:E:573:VAL:HG12 | 1.97                     | 0.64              |
| 1:E:601:LYS:HB2  | 1:E:603:ILE:HG13 | 1.79                     | 0.64              |
| 1:E:651:PHE:HB2  | 1:E:688:ALA:CB   | 2.27                     | 0.64              |
| 1:E:749:VAL:O    | 1:E:753:GLN:HG3  | 1.97                     | 0.64              |
| 1:F:729:VAL:HG11 | 1:F:735:ASN:HB3  | 1.78                     | 0.64              |
| 1:A:200:GLY:C    | 1:A:202:PRO:HD2  | 2.18                     | 0.64              |
| 1:B:219:LYS:HA   | 1:B:224:ILE:HB   | 1.77                     | 0.64              |
| 1:B:456:ILE:HD11 | 1:B:479:VAL:HB   | 1.79                     | 0.64              |
| 1:C:292:LEU:HD12 | 1:C:296:LEU:HD21 | 1.79                     | 0.64              |
| 1:C:405:ALA:O    | 1:C:466:THR:HG21 | 1.97                     | 0.64              |
| 1:E:224:ILE:HG13 | 1:E:338:VAL:HG13 | 1.78                     | 0.64              |
| 1:B:491:ILE:HD12 | 1:B:525:LEU:HD12 | 1.78                     | 0.64              |
| 1:C:37:LEU:HD23  | 1:C:40:ALA:O     | 1.98                     | 0.64              |
| 1:C:50:GLU:O     | 1:C:53:ILE:HG22  | 1.97                     | 0.64              |
| 1:D:564:VAL:HG13 | 1:D:667:GLN:HE21 | 1.62                     | 0.64              |
| 1:E:18:ARG:HH22  | 1:E:36:ASN:ND2   | 1.96                     | 0.64              |
| 1:F:687:LEU:CD2  | 1:F:724:MSE:HB2  | 2.27                     | 0.64              |
| 1:A:653:VAL:HG13 | 1:A:692:ALA:HB3  | 1.80                     | 0.64              |
| 1:A:475:ASN:ND2  | 1:B:591:GLU:HG2  | 2.10                     | 0.64              |
| 1:C:312:THR:O    | 1:C:315:ILE:HG22 | 1.98                     | 0.64              |
| 1:D:491:ILE:HG23 | 1:D:527:LEU:HD11 | 1.80                     | 0.64              |
| 1:D:690:ALA:O    | 1:D:725:ILE:HG12 | 1.97                     | 0.64              |
| 1:F:456:ILE:HG22 | 1:F:457:ILE:H    | 1.61                     | 0.64              |
| 1:A:232:ASN:HB3  | 1:A:235:VAL:HG22 | 1.79                     | 0.64              |
| 1:A:292:LEU:HD11 | 1:A:324:VAL:HG21 | 1.80                     | 0.64              |
| 1:A:451:LYS:HA   | 1:A:477:LEU:HD21 | 1.79                     | 0.64              |
| 1:C:409:ASN:ND2  | 1:C:425:ILE:HD11 | 2.12                     | 0.64              |
| 1:E:519:THR:HB   | 1:E:608:ALA:HA   | 1.79                     | 0.64              |
| 1:E:521:GLY:HA3  | 1:E:610:SER:HA   | 1.79                     | 0.64              |
| 1:C:601:LYS:NZ   | 1:F:771:MSE:HE3  | 2.13                     | 0.64              |
| 1:C:188:TYR:CZ   | 1:C:312:THR:HG21 | 2.32                     | 0.64              |
| 1:F:581:ALA:HA   | 1:F:584:SER:HB3  | 1.80                     | 0.64              |
| 1:A:183:VAL:CG2  | 1:A:184:CYS:N    | 2.61                     | 0.64              |
| 1:C:192:THR:C    | 1:C:194:ASP:H    | 1.99                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:437:MSE:O    | 1:C:441:ILE:HG13 | 1.98                     | 0.64              |
| 1:F:32:GLY:H     | 1:F:87:TYR:HD2   | 1.44                     | 0.64              |
| 1:F:380:VAL:HG12 | 1:F:381:ILE:N    | 2.12                     | 0.64              |
| 1:B:163:ARG:HB2  | 1:B:163:ARG:NH1  | 2.12                     | 0.64              |
| 1:B:549:ALA:HA   | 1:B:555:ARG:HB2  | 1.78                     | 0.64              |
| 1:C:583:GLU:H    | 1:C:583:GLU:CD   | 2.01                     | 0.64              |
| 1:F:142:GLU:HB3  | 1:F:150:ASN:O    | 1.98                     | 0.64              |
| 1:A:282:ILE:HG13 | 1:A:283:THR:H    | 1.63                     | 0.64              |
| 1:B:544:PRO:HB2  | 1:B:555:ARG:NH2  | 2.13                     | 0.64              |
| 1:B:6:ILE:HG23   | 1:B:73:ILE:HG23  | 1.80                     | 0.64              |
| 1:C:394:ILE:HD11 | 1:C:419:VAL:HB   | 1.80                     | 0.64              |
| 1:D:216:VAL:HG23 | 1:D:354:TYR:C    | 2.18                     | 0.64              |
| 1:F:651:PHE:HB2  | 1:F:688:ALA:CB   | 2.28                     | 0.64              |
| 1:F:57:ILE:HG13  | 1:F:75:LYS:HZ3   | 1.61                     | 0.64              |
| 1:A:49:ARG:CD    | 1:A:49:ARG:H     | 2.09                     | 0.63              |
| 1:A:633:GLU:N    | 1:A:634:PRO:HD2  | 2.14                     | 0.63              |
| 1:A:759:LEU:HD22 | 1:A:765:LEU:HB2  | 1.79                     | 0.63              |
| 1:A:757:GLY:O    | 1:A:760:TYR:HB3  | 1.98                     | 0.63              |
| 1:D:524:VAL:HG23 | 1:D:536:ALA:H    | 1.62                     | 0.63              |
| 1:F:427:ASN:O    | 1:F:433:VAL:HG21 | 1.98                     | 0.63              |
| 1:A:615:LEU:HD11 | 1:A:635:ALA:HA   | 1.81                     | 0.63              |
| 1:C:12:VAL:HG13  | 1:C:13:GLN:H     | 1.61                     | 0.63              |
| 1:C:338:VAL:HG23 | 1:C:343:ARG:HB2  | 1.79                     | 0.63              |
| 1:D:232:ASN:HB3  | 1:D:235:VAL:HG22 | 1.80                     | 0.63              |
| 1:E:127:PRO:HB3  | 1:E:312:THR:CG2  | 2.27                     | 0.63              |
| 1:E:502:SER:HB3  | 1:E:528:GLY:HA2  | 1.80                     | 0.63              |
| 1:A:752:GLY:O    | 1:A:756:LEU:HB2  | 1.97                     | 0.63              |
| 1:B:369:SER:HB2  | 1:B:385:ARG:HB2  | 1.81                     | 0.63              |
| 1:D:161:PHE:O    | 1:D:164:SER:HB2  | 1.97                     | 0.63              |
| 1:D:529:TYR:HD1  | 1:D:764:TYR:HB3  | 1.63                     | 0.63              |
| 1:F:373:PHE:CE2  | 1:F:378:ARG:HD3  | 2.34                     | 0.63              |
| 1:F:549:ALA:HA   | 1:F:555:ARG:HB2  | 1.80                     | 0.63              |
| 1:B:270:GLU:HB2  | 1:B:373:PHE:HE2  | 1.64                     | 0.63              |
| 1:B:584:SER:HB3  | 1:B:589:LYS:HB3  | 1.80                     | 0.63              |
| 1:E:380:VAL:HG12 | 1:E:381:ILE:H    | 1.63                     | 0.63              |
| 1:A:17:PHE:O     | 1:A:21:VAL:HG23  | 1.97                     | 0.63              |
| 1:A:485:GLN:OE1  | 1:A:514:GLY:HA2  | 1.99                     | 0.63              |
| 1:D:653:VAL:HG11 | 1:D:689:LEU:HD12 | 1.79                     | 0.63              |
| 1:F:221:ILE:HA   | 1:F:360:ARG:HH22 | 1.64                     | 0.63              |
| 1:F:263:PHE:HZ   | 1:F:303:ILE:HG21 | 1.62                     | 0.63              |
| 1:F:589:LYS:HG3  | 1:F:590:VAL:N    | 2.12                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:201:ASP:N    | 1:A:202:PRO:CD   | 2.61                     | 0.63              |
| 1:B:215:ILE:HG22 | 1:B:228:CYS:HB2  | 1.81                     | 0.63              |
| 1:B:566:SER:H    | 1:B:569:GLU:HB2  | 1.63                     | 0.63              |
| 1:B:580:LYS:HE2  | 1:B:593:ASN:ND2  | 2.13                     | 0.63              |
| 1:D:219:LYS:HG2  | 1:D:358:HIS:NE2  | 2.13                     | 0.63              |
| 1:F:126:TYR:CZ   | 1:F:128:PHE:HB2  | 2.34                     | 0.63              |
| 1:A:108:ILE:HG13 | 1:A:311:GLY:H    | 1.63                     | 0.63              |
| 1:B:265:TYR:O    | 1:B:284:LEU:HD22 | 1.98                     | 0.63              |
| 1:F:396:PHE:CE2  | 1:F:759:LEU:HB2  | 2.34                     | 0.63              |
| 1:E:760:TYR:HE2  | 1:E:767:LYS:HG2  | 1.64                     | 0.63              |
| 1:F:224:ILE:HD13 | 1:F:357:LEU:HD22 | 1.81                     | 0.63              |
| 1:A:114:ARG:O    | 1:A:118:ASP:HB2  | 1.98                     | 0.63              |
| 1:A:369:SER:H    | 1:A:385:ARG:HB2  | 1.64                     | 0.63              |
| 1:A:629:HIS:HB2  | 1:A:633:GLU:OE1  | 1.98                     | 0.63              |
| 1:A:590:VAL:N    | 1:B:475:ASN:HD21 | 1.96                     | 0.63              |
| 1:B:501:ASP:O    | 1:B:503:VAL:HG13 | 1.99                     | 0.63              |
| 1:C:13:GLN:NE2   | 1:C:42:VAL:HG23  | 2.13                     | 0.63              |
| 1:D:434:LEU:HD13 | 1:D:465:ASN:HB3  | 1.81                     | 0.63              |
| 1:D:742:VAL:HG11 | 1:D:751:VAL:HG11 | 1.81                     | 0.63              |
| 1:D:88:ILE:CG2   | 1:D:89:GLU:H     | 2.09                     | 0.63              |
| 1:F:239:LEU:O    | 1:F:239:LEU:HD23 | 1.98                     | 0.63              |
| 1:F:613:ARG:HE   | 1:F:613:ARG:HA   | 1.64                     | 0.63              |
| 1:A:5:HIS:HB3    | 1:A:76:LYS:HB2   | 1.80                     | 0.62              |
| 1:B:210:ILE:HD11 | 1:B:228:CYS:N    | 2.13                     | 0.62              |
| 1:B:566:SER:N    | 1:B:569:GLU:HB2  | 2.14                     | 0.62              |
| 1:C:253:MSE:O    | 1:C:324:VAL:HA   | 1.98                     | 0.62              |
| 1:F:137:ARG:HH22 | 1:F:178:PRO:HG3  | 1.62                     | 0.62              |
| 1:A:148:ARG:CZ   | 1:A:158:MSE:HG3  | 2.28                     | 0.62              |
| 1:B:374:VAL:HG11 | 1:B:744:ARG:HH22 | 1.64                     | 0.62              |
| 1:B:651:PHE:HE2  | 1:B:669:ILE:HA   | 1.63                     | 0.62              |
| 1:C:261:LYS:HZ3  | 1:C:266:VAL:HB   | 1.63                     | 0.62              |
| 1:F:430:LYS:HB2  | 1:F:433:VAL:HG23 | 1.80                     | 0.62              |
| 1:F:697:ALA:HB1  | 1:F:709:VAL:HG11 | 1.80                     | 0.62              |
| 1:C:239:LEU:O    | 1:C:243:THR:HG22 | 1.98                     | 0.62              |
| 1:F:264:ALA:HB2  | 1:F:286:LYS:HA   | 1.80                     | 0.62              |
| 1:F:620:VAL:HG13 | 1:F:626:TYR:HD1  | 1.64                     | 0.62              |
| 1:F:665:LEU:HD22 | 1:F:689:LEU:HD13 | 1.81                     | 0.62              |
| 1:A:20:PHE:O     | 1:A:24:ILE:HG22  | 1.99                     | 0.62              |
| 1:A:329:SER:HB2  | 1:A:331:ASN:HD21 | 1.64                     | 0.62              |
| 1:A:494:VAL:HG22 | 1:A:738:VAL:HG22 | 1.80                     | 0.62              |
| 1:B:8:VAL:HG11   | 1:B:12:VAL:HG21  | 1.81                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:373:PHE:CD1  | 1:B:378:ARG:HB3  | 2.35                     | 0.62              |
| 1:A:708:ASN:HB3  | 1:A:734:LEU:O    | 1.99                     | 0.62              |
| 1:A:497:GLU:OE2  | 1:A:741:GLU:HB3  | 2.00                     | 0.62              |
| 1:C:281:ILE:HB   | 1:C:370:VAL:CG1  | 2.25                     | 0.62              |
| 1:C:104:PRO:HD3  | 1:C:390:LEU:HD21 | 1.82                     | 0.62              |
| 1:D:226:LEU:HD11 | 1:D:348:LEU:HD23 | 1.81                     | 0.62              |
| 1:D:385:ARG:HG3  | 1:D:386:GLY:N    | 2.14                     | 0.62              |
| 1:D:408:MSE:HG3  | 1:D:424:TYR:CE1  | 2.34                     | 0.62              |
| 1:D:553:PRO:CD   | 1:D:627:ARG:HA   | 2.30                     | 0.62              |
| 1:D:649:LEU:HD12 | 1:D:650:LYS:H    | 1.64                     | 0.62              |
| 1:E:66:PRO:HD2   | 1:E:133:ASN:ND2  | 2.15                     | 0.62              |
| 1:E:5:HIS:HB3    | 1:E:76:LYS:HB2   | 1.80                     | 0.62              |
| 1:F:329:SER:HB2  | 1:F:331:ASN:HD21 | 1.65                     | 0.62              |
| 1:A:116:LEU:HB3  | 1:A:129:ILE:HD12 | 1.80                     | 0.62              |
| 1:A:325:TYR:O    | 1:A:326:VAL:HG23 | 2.00                     | 0.62              |
| 1:B:281:ILE:HG12 | 1:B:306:MSE:HG2  | 1.80                     | 0.62              |
| 1:C:219:LYS:HE3  | 1:C:358:HIS:CE1  | 2.35                     | 0.62              |
| 1:D:282:ILE:HD12 | 1:D:371:ILE:O    | 1.99                     | 0.62              |
| 1:D:373:PHE:CE1  | 1:D:378:ARG:HB3  | 2.34                     | 0.62              |
| 1:E:370:VAL:H    | 1:E:382:ARG:HB3  | 1.64                     | 0.62              |
| 1:F:729:VAL:HB   | 1:F:735:ASN:HD22 | 1.65                     | 0.62              |
| 1:A:534:ARG:HG2  | 1:A:535:LEU:N    | 2.14                     | 0.62              |
| 1:B:225:HIS:HB2  | 1:B:328:THR:O    | 2.00                     | 0.62              |
| 1:C:258:GLU:HG3  | 1:C:259:THR:H    | 1.61                     | 0.62              |
| 1:C:534:ARG:HD3  | 1:C:537:HIS:HD2  | 1.65                     | 0.62              |
| 1:D:105:ASP:OD1  | 1:D:139:THR:HG23 | 1.99                     | 0.62              |
| 1:F:193:SER:O    | 1:F:194:ASP:HB2  | 2.00                     | 0.62              |
| 1:F:464:TYR:HB2  | 1:F:467:THR:HG23 | 1.80                     | 0.62              |
| 1:F:590:VAL:O    | 1:F:594:VAL:HG23 | 2.00                     | 0.62              |
| 1:A:475:ASN:ND2  | 1:B:589:LYS:H    | 1.98                     | 0.62              |
| 1:C:570:LEU:O    | 1:C:573:VAL:HG12 | 2.00                     | 0.62              |
| 1:C:649:LEU:HD12 | 1:C:650:LYS:H    | 1.64                     | 0.62              |
| 1:D:408:MSE:HG3  | 1:D:424:TYR:HE1  | 1.64                     | 0.62              |
| 1:E:111:ASP:HB3  | 1:E:172:ARG:NH2  | 2.15                     | 0.62              |
| 1:E:142:GLU:HB3  | 1:E:150:ASN:O    | 1.99                     | 0.62              |
| 1:E:168:ASP:O    | 1:E:174:TYR:HB2  | 2.00                     | 0.62              |
| 1:A:210:ILE:HD11 | 1:A:228:CYS:N    | 2.14                     | 0.62              |
| 1:A:263:PHE:HZ   | 1:A:303:ILE:HG21 | 1.64                     | 0.62              |
| 1:A:65:PRO:HG2   | 1:A:68:ALA:HB3   | 1.80                     | 0.62              |
| 1:A:749:VAL:O    | 1:A:753:GLN:HG3  | 2.00                     | 0.62              |
| 1:B:1:MSE:HG2    | 1:B:83:PHE:HD1   | 1.65                     | 0.62              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:169:PRO:HG2  | 1:C:170:LEU:HD12 | 1.81                     | 0.62              |
| 1:C:422:SER:HA   | 1:C:444:PHE:CZ   | 2.34                     | 0.62              |
| 1:C:495:MSE:SE   | 1:C:527:LEU:HD13 | 2.50                     | 0.62              |
| 1:E:210:ILE:HD11 | 1:E:228:CYS:CA   | 2.28                     | 0.62              |
| 1:E:380:VAL:HG12 | 1:E:381:ILE:N    | 2.15                     | 0.62              |
| 1:A:521:GLY:CA   | 1:A:610:SER:HA   | 2.30                     | 0.62              |
| 1:C:253:MSE:HA   | 1:C:306:MSE:O    | 2.00                     | 0.62              |
| 1:D:543:LEU:N    | 1:D:543:LEU:HD23 | 2.13                     | 0.62              |
| 1:F:190:LEU:HG   | 1:F:202:PRO:CB   | 2.29                     | 0.62              |
| 1:F:65:PRO:HG2   | 1:F:68:ALA:HB3   | 1.82                     | 0.62              |
| 1:A:580:LYS:HG3  | 1:A:593:ASN:HD22 | 1.65                     | 0.61              |
| 1:B:498:LYS:HB2  | 1:B:500:LEU:CD2  | 2.29                     | 0.61              |
| 1:C:603:ILE:HG23 | 1:F:516:ASP:HA   | 1.81                     | 0.61              |
| 1:C:756:LEU:HD22 | 1:C:770:LEU:HD21 | 1.82                     | 0.61              |
| 1:D:590:VAL:O    | 1:D:594:VAL:HG23 | 1.99                     | 0.61              |
| 1:D:61:TYR:OH    | 1:D:73:ILE:HD12  | 1.99                     | 0.61              |
| 1:E:737:HIS:HB3  | 1:E:744:ARG:HD3  | 1.82                     | 0.61              |
| 1:F:583:GLU:HG3  | 1:F:592:PHE:CD1  | 2.35                     | 0.61              |
| 1:A:236:VAL:HG13 | 1:A:295:ASN:ND2  | 2.15                     | 0.61              |
| 1:B:525:LEU:HD23 | 1:B:534:ARG:HA   | 1.81                     | 0.61              |
| 1:C:224:ILE:HG23 | 1:C:338:VAL:HG13 | 1.82                     | 0.61              |
| 1:D:543:LEU:HD12 | 1:D:549:ALA:HB3  | 1.82                     | 0.61              |
| 1:E:201:ASP:N    | 1:E:202:PRO:CD   | 2.63                     | 0.61              |
| 1:E:204:ARG:HG2  | 1:E:319:TRP:CE2  | 2.35                     | 0.61              |
| 1:E:394:ILE:CD1  | 1:E:419:VAL:HB   | 2.28                     | 0.61              |
| 1:E:445:ARG:HH21 | 1:E:452:ASN:ND2  | 1.97                     | 0.61              |
| 1:E:61:TYR:CZ    | 1:E:73:ILE:HD12  | 2.34                     | 0.61              |
| 1:C:226:LEU:HD21 | 1:C:351:VAL:HG12 | 1.81                     | 0.61              |
| 1:C:138:PHE:HB2  | 1:C:389:PRO:HD3  | 1.82                     | 0.61              |
| 1:D:8:VAL:O      | 1:D:9:GLN:HG3    | 2.00                     | 0.61              |
| 1:E:111:ASP:CB   | 1:E:172:ARG:HH22 | 2.14                     | 0.61              |
| 1:F:385:ARG:HG3  | 1:F:386:GLY:H    | 1.64                     | 0.61              |
| 1:F:498:LYS:HE3  | 1:F:736:PHE:HB2  | 1.83                     | 0.61              |
| 1:B:502:SER:CB   | 1:B:528:GLY:HA2  | 2.29                     | 0.61              |
| 1:D:553:PRO:HD2  | 1:D:627:ARG:HA   | 1.82                     | 0.61              |
| 1:E:391:PRO:HB2  | 1:E:418:LYS:HB2  | 1.82                     | 0.61              |
| 1:F:255:LYS:HB2  | 1:F:323:PRO:CB   | 2.29                     | 0.61              |
| 1:B:743:PRO:HG3  | 1:B:747:ASN:HD21 | 1.66                     | 0.61              |
| 1:C:196:GLN:HG2  | 1:C:197:GLU:N    | 2.15                     | 0.61              |
| 1:E:47:GLU:CB    | 1:E:80:PRO:HG2   | 2.30                     | 0.61              |
| 1:A:216:VAL:HB   | 1:A:354:TYR:HB2  | 1.82                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:258:GLU:CG   | 1:C:259:THR:N    | 2.62                     | 0.61              |
| 1:D:427:ASN:ND2  | 1:D:429:GLY:H    | 1.98                     | 0.61              |
| 1:D:601:LYS:HB2  | 1:D:603:ILE:HG13 | 1.82                     | 0.61              |
| 1:E:485:GLN:OE1  | 1:E:514:GLY:HA2  | 2.01                     | 0.61              |
| 1:F:292:LEU:HD11 | 1:F:324:VAL:HG21 | 1.82                     | 0.61              |
| 1:A:282:ILE:HG13 | 1:A:283:THR:N    | 2.16                     | 0.61              |
| 1:B:125:MSE:O    | 1:B:127:PRO:HD3  | 2.01                     | 0.61              |
| 1:B:313:HIS:HE1  | 1:B:327:MSE:HE2  | 1.64                     | 0.61              |
| 1:B:485:GLN:CG   | 1:B:488:TYR:H    | 2.12                     | 0.61              |
| 1:C:232:ASN:OD1  | 1:C:234:GLU:HB3  | 2.00                     | 0.61              |
| 1:D:257:ILE:HD12 | 1:D:260:VAL:HG21 | 1.83                     | 0.61              |
| 1:E:489:ALA:O    | 1:E:492:ALA:HB3  | 2.00                     | 0.61              |
| 1:F:690:ALA:HB1  | 1:F:725:ILE:HG13 | 1.83                     | 0.61              |
| 1:B:380:VAL:HG12 | 1:B:381:ILE:N    | 2.16                     | 0.61              |
| 1:C:614:VAL:O    | 1:C:618:ILE:HG13 | 2.01                     | 0.61              |
| 1:F:106:ILE:CG2  | 1:F:277:TYR:HB2  | 2.30                     | 0.61              |
| 1:F:61:TYR:OH    | 1:F:73:ILE:HD12  | 2.00                     | 0.61              |
| 1:B:491:ILE:HG22 | 1:B:527:LEU:HD11 | 1.81                     | 0.61              |
| 1:A:727:LYS:NZ   | 1:C:287:LYS:HE3  | 2.15                     | 0.61              |
| 1:E:670:LEU:O    | 1:E:673:ILE:HG12 | 2.01                     | 0.61              |
| 1:F:154:LYS:HD3  | 1:F:154:LYS:O    | 2.01                     | 0.61              |
| 1:F:15:VAL:HG22  | 1:F:103:PRO:HB3  | 1.82                     | 0.61              |
| 1:F:183:VAL:HG23 | 1:F:184:CYS:N    | 2.16                     | 0.61              |
| 1:F:17:PHE:O     | 1:F:21:VAL:HG23  | 2.00                     | 0.61              |
| 1:F:633:GLU:N    | 1:F:634:PRO:HD2  | 2.16                     | 0.61              |
| 1:C:584:SER:HB3  | 1:C:589:LYS:HB3  | 1.83                     | 0.61              |
| 1:D:111:ASP:CB   | 1:D:172:ARG:HH22 | 2.10                     | 0.61              |
| 1:F:614:VAL:O    | 1:F:618:ILE:HG13 | 2.01                     | 0.61              |
| 1:A:123:ARG:NH2  | 1:A:173:ARG:HE   | 1.98                     | 0.60              |
| 1:A:590:VAL:O    | 1:A:594:VAL:HG23 | 2.01                     | 0.60              |
| 1:B:200:GLY:C    | 1:B:202:PRO:HD2  | 2.21                     | 0.60              |
| 1:C:450:VAL:HG22 | 1:C:451:LYS:H    | 1.66                     | 0.60              |
| 1:C:759:LEU:CD1  | 1:C:764:TYR:HB2  | 2.30                     | 0.60              |
| 1:D:369:SER:N    | 1:D:385:ARG:HB2  | 2.10                     | 0.60              |
| 1:D:542:PRO:HD3  | 1:D:563:LYS:HE2  | 1.82                     | 0.60              |
| 1:F:370:VAL:H    | 1:F:382:ARG:HB3  | 1.65                     | 0.60              |
| 1:A:142:GLU:HB3  | 1:A:150:ASN:O    | 2.00                     | 0.60              |
| 1:A:49:ARG:O     | 1:A:53:ILE:HB    | 2.01                     | 0.60              |
| 1:A:572:GLY:HA2  | 1:A:575:ASN:HD22 | 1.67                     | 0.60              |
| 1:A:698:VAL:HG13 | 1:A:732:ASN:HD22 | 1.65                     | 0.60              |
| 1:C:456:ILE:HG22 | 1:C:457:ILE:N    | 2.16                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:282:ILE:HG13 | 1:D:283:THR:N    | 2.16                     | 0.60              |
| 1:D:456:ILE:HG22 | 1:D:457:ILE:N    | 2.16                     | 0.60              |
| 1:F:506:ILE:O    | 1:F:711:LEU:HD12 | 2.00                     | 0.60              |
| 1:F:35:LYS:HE2   | 1:F:90:LYS:NZ    | 2.14                     | 0.60              |
| 1:D:270:GLU:HB2  | 1:D:373:PHE:HE2  | 1.66                     | 0.60              |
| 1:E:500:LEU:HD13 | 1:E:736:PHE:CZ   | 2.36                     | 0.60              |
| 1:F:649:LEU:HB3  | 1:F:684:SER:CB   | 2.31                     | 0.60              |
| 1:A:524:VAL:HG22 | 1:A:536:ALA:CB   | 2.31                     | 0.60              |
| 1:B:394:ILE:CD1  | 1:B:419:VAL:HB   | 2.25                     | 0.60              |
| 1:B:729:VAL:CB   | 1:B:735:ASN:HD22 | 2.14                     | 0.60              |
| 1:C:373:PHE:CE2  | 1:C:378:ARG:HD3  | 2.37                     | 0.60              |
| 1:C:504:ILE:O    | 1:C:709:VAL:HA   | 2.01                     | 0.60              |
| 1:E:691:ARG:NE   | 1:E:724:MSE:HE2  | 2.14                     | 0.60              |
| 1:F:469:LEU:O    | 1:F:473:MSE:HB2  | 2.01                     | 0.60              |
| 1:A:616:ASP:CG   | 1:A:634:PRO:HG3  | 2.22                     | 0.60              |
| 1:C:759:LEU:HD11 | 1:C:764:TYR:HB2  | 1.83                     | 0.60              |
| 1:D:144:LEU:HD23 | 1:D:146:TYR:H    | 1.67                     | 0.60              |
| 1:D:148:ARG:O    | 1:D:151:THR:HG22 | 2.01                     | 0.60              |
| 1:D:253:MSE:O    | 1:D:324:VAL:HA   | 2.02                     | 0.60              |
| 1:E:266:VAL:HG13 | 1:E:270:GLU:OE2  | 2.01                     | 0.60              |
| 1:E:286:LYS:HE3  | 1:E:290:PHE:HB2  | 1.84                     | 0.60              |
| 1:E:406:GLU:HG3  | 1:E:407:LEU:HG   | 1.82                     | 0.60              |
| 1:F:287:LYS:HG3  | 1:F:289:PRO:HD2  | 1.83                     | 0.60              |
| 1:A:239:LEU:O    | 1:A:243:THR:HG22 | 2.02                     | 0.60              |
| 1:A:15:VAL:HG21  | 1:A:67:LEU:O     | 2.02                     | 0.60              |
| 1:B:373:PHE:CE2  | 1:B:378:ARG:HD3  | 2.36                     | 0.60              |
| 1:B:408:MSE:HG3  | 1:B:424:TYR:CE1  | 2.37                     | 0.60              |
| 1:D:504:ILE:O    | 1:D:709:VAL:HA   | 2.01                     | 0.60              |
| 1:D:572:GLY:HA2  | 1:D:575:ASN:HD22 | 1.66                     | 0.60              |
| 1:D:665:LEU:HD22 | 1:D:689:LEU:HD13 | 1.83                     | 0.60              |
| 1:E:257:ILE:HD12 | 1:E:260:VAL:HB   | 1.83                     | 0.60              |
| 1:E:759:LEU:HD11 | 1:E:764:TYR:HB2  | 1.83                     | 0.60              |
| 1:B:263:PHE:CZ   | 1:B:303:ILE:HG21 | 2.36                     | 0.60              |
| 1:B:35:LYS:HG3   | 1:B:90:LYS:HD2   | 1.83                     | 0.60              |
| 1:B:759:LEU:HD11 | 1:B:764:TYR:HB2  | 1.84                     | 0.60              |
| 1:C:552:TYR:HE1  | 1:C:627:ARG:NE   | 1.99                     | 0.60              |
| 1:B:158:MSE:HE3  | 1:B:163:ARG:CZ   | 2.32                     | 0.60              |
| 1:B:401:LEU:HD12 | 1:B:402:ALA:H    | 1.67                     | 0.60              |
| 1:B:620:VAL:C    | 1:B:622:LEU:H    | 2.05                     | 0.60              |
| 1:C:485:GLN:CB   | 1:C:488:TYR:HB2  | 2.32                     | 0.60              |
| 1:E:9:GLN:HB2    | 1:E:72:ARG:HD2   | 1.84                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:6:ILE:HD12   | 1:E:73:ILE:HG23  | 1.82                     | 0.60              |
| 1:F:405:ALA:O    | 1:F:466:THR:HG21 | 2.01                     | 0.60              |
| 1:A:282:ILE:HD12 | 1:A:371:ILE:O    | 2.02                     | 0.60              |
| 1:A:634:PRO:HG2  | 1:A:635:ALA:H    | 1.67                     | 0.60              |
| 1:B:653:VAL:HG13 | 1:B:692:ALA:CB   | 2.30                     | 0.60              |
| 1:C:204:ARG:HG2  | 1:C:319:TRP:CZ2  | 2.37                     | 0.60              |
| 1:D:371:ILE:CD1  | 1:D:380:VAL:HG22 | 2.31                     | 0.60              |
| 1:E:30:LEU:HG    | 1:E:48:GLY:HA3   | 1.84                     | 0.60              |
| 1:A:299:GLY:O    | 1:A:300:LEU:HG   | 2.02                     | 0.60              |
| 1:A:587:TYR:HD1  | 1:A:588:GLY:N    | 1.93                     | 0.60              |
| 1:B:274:LEU:HB3  | 1:B:307:LEU:HD11 | 1.84                     | 0.60              |
| 1:B:540:TYR:HD1  | 1:B:540:TYR:H    | 1.48                     | 0.60              |
| 1:D:409:ASN:ND2  | 1:D:425:ILE:HD11 | 2.17                     | 0.60              |
| 1:D:34:VAL:O     | 1:D:89:GLU:HA    | 2.02                     | 0.60              |
| 1:E:281:ILE:HG12 | 1:E:306:MSE:HG2  | 1.83                     | 0.60              |
| 1:E:726:ARG:HH21 | 1:E:727:LYS:HG2  | 1.67                     | 0.60              |
| 1:A:445:ARG:HH21 | 1:A:452:ASN:ND2  | 2.00                     | 0.59              |
| 1:B:504:ILE:HG22 | 1:B:505:GLY:N    | 2.16                     | 0.59              |
| 1:C:409:ASN:O    | 1:C:425:ILE:HG12 | 2.02                     | 0.59              |
| 1:D:554:LEU:HD11 | 1:D:579:PRO:HB2  | 1.83                     | 0.59              |
| 1:E:554:LEU:O    | 1:E:558:MSE:HG3  | 2.02                     | 0.59              |
| 1:F:371:ILE:HD11 | 1:F:373:PHE:HE1  | 1.67                     | 0.59              |
| 1:F:445:ARG:HH21 | 1:F:452:ASN:HD22 | 1.48                     | 0.59              |
| 1:A:405:ALA:O    | 1:A:466:THR:HG21 | 2.02                     | 0.59              |
| 1:A:144:LEU:HD12 | 1:A:447:ILE:HG23 | 1.83                     | 0.59              |
| 1:B:312:THR:O    | 1:B:315:ILE:HG22 | 2.02                     | 0.59              |
| 1:B:219:LYS:HD3  | 1:B:358:HIS:H    | 1.66                     | 0.59              |
| 1:B:425:ILE:HG22 | 1:B:436:PHE:CE1  | 2.38                     | 0.59              |
| 1:A:723:LYS:HE2  | 1:C:289:PRO:HG2  | 1.83                     | 0.59              |
| 1:C:524:VAL:HG22 | 1:C:536:ALA:HB3  | 1.82                     | 0.59              |
| 1:D:526:TYR:HB2  | 1:D:535:LEU:HD11 | 1.85                     | 0.59              |
| 1:D:566:SER:N    | 1:D:569:GLU:HB2  | 2.13                     | 0.59              |
| 1:E:261:LYS:HZ3  | 1:E:266:VAL:HB   | 1.67                     | 0.59              |
| 1:E:329:SER:HB2  | 1:E:331:ASN:ND2  | 2.17                     | 0.59              |
| 1:A:196:GLN:HG2  | 1:A:197:GLU:O    | 2.01                     | 0.59              |
| 1:A:553:PRO:HG3  | 1:A:626:TYR:O    | 2.01                     | 0.59              |
| 1:B:391:PRO:HB3  | 1:B:420:TYR:CE1  | 2.38                     | 0.59              |
| 1:C:171:ASN:ND2  | 1:C:173:ARG:HB2  | 2.18                     | 0.59              |
| 1:C:215:ILE:HG22 | 1:C:228:CYS:HB2  | 1.83                     | 0.59              |
| 1:C:225:HIS:HA   | 1:C:330:ALA:CB   | 2.32                     | 0.59              |
| 1:D:144:LEU:HD23 | 1:D:146:TYR:N    | 2.17                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:166:TYR:CE1  | 1:D:175:HIS:HA   | 2.38                     | 0.59              |
| 1:D:614:VAL:O    | 1:D:618:ILE:HG13 | 2.02                     | 0.59              |
| 1:E:156:PHE:CZ   | 1:E:186:PRO:HB3  | 2.38                     | 0.59              |
| 1:E:396:PHE:CE2  | 1:E:759:LEU:HB2  | 2.36                     | 0.59              |
| 1:F:370:VAL:HG23 | 1:F:381:ILE:HD11 | 1.83                     | 0.59              |
| 1:A:253:MSE:HE2  | 1:A:317:PHE:CD1  | 2.37                     | 0.59              |
| 1:A:554:LEU:O    | 1:A:558:MSE:HG3  | 2.02                     | 0.59              |
| 1:B:107:ALA:O    | 1:B:134:CYS:HB2  | 2.02                     | 0.59              |
| 1:C:554:LEU:O    | 1:C:558:MSE:HG3  | 2.03                     | 0.59              |
| 1:C:724:MSE:O    | 1:C:728:VAL:HG23 | 2.03                     | 0.59              |
| 1:D:468:LYS:HG3  | 1:E:587:TYR:OH   | 2.03                     | 0.59              |
| 1:D:654:PRO:HG3  | 1:D:664:GLU:OE1  | 2.02                     | 0.59              |
| 1:E:456:ILE:HG22 | 1:E:457:ILE:N    | 2.18                     | 0.59              |
| 1:E:419:VAL:HG11 | 1:E:751:VAL:HG23 | 1.83                     | 0.59              |
| 1:F:601:LYS:HB2  | 1:F:603:ILE:HG13 | 1.83                     | 0.59              |
| 1:A:247:GLN:HG3  | 1:A:298:PRO:HG2  | 1.83                     | 0.59              |
| 1:B:15:VAL:HG12  | 1:B:16:GLY:H     | 1.68                     | 0.59              |
| 1:B:239:LEU:O    | 1:B:239:LEU:HD23 | 2.03                     | 0.59              |
| 1:C:406:GLU:HG3  | 1:C:407:LEU:N    | 2.16                     | 0.59              |
| 1:D:171:ASN:ND2  | 1:D:173:ARG:H    | 2.00                     | 0.59              |
| 1:E:464:TYR:HB2  | 1:E:467:THR:HG23 | 1.84                     | 0.59              |
| 1:F:106:ILE:HG23 | 1:F:277:TYR:HB2  | 1.84                     | 0.59              |
| 1:A:267:SER:H    | 1:A:270:GLU:CD   | 2.06                     | 0.59              |
| 1:B:282:ILE:HG23 | 1:B:283:THR:N    | 2.15                     | 0.59              |
| 1:B:751:VAL:HG13 | 1:B:752:GLY:N    | 2.17                     | 0.59              |
| 1:C:526:TYR:O    | 1:C:532:VAL:HG13 | 2.03                     | 0.59              |
| 1:C:66:PRO:HG3   | 1:C:133:ASN:HB3  | 1.85                     | 0.59              |
| 1:D:383:ARG:HB3  | 1:D:747:ASN:HD21 | 1.68                     | 0.59              |
| 1:D:398:TYR:HB2  | 1:D:454:ASP:OD2  | 2.03                     | 0.59              |
| 1:E:543:LEU:HD12 | 1:E:549:ALA:HB3  | 1.85                     | 0.59              |
| 1:E:572:GLY:HA2  | 1:E:575:ASN:ND2  | 2.17                     | 0.59              |
| 1:E:729:VAL:HB   | 1:E:735:ASN:HD22 | 1.66                     | 0.59              |
| 1:F:254:ALA:HB1  | 1:F:259:THR:HB   | 1.85                     | 0.59              |
| 1:F:265:TYR:CE2  | 1:F:287:LYS:HD2  | 2.31                     | 0.59              |
| 1:F:370:VAL:CG2  | 1:F:381:ILE:HD11 | 2.33                     | 0.59              |
| 1:B:281:ILE:HG12 | 1:B:306:MSE:CG   | 2.33                     | 0.59              |
| 1:B:374:VAL:CG2  | 1:B:744:ARG:HH22 | 2.14                     | 0.59              |
| 1:D:137:ARG:HH22 | 1:D:178:PRO:HG3  | 1.67                     | 0.59              |
| 1:E:210:ILE:CD1  | 1:E:228:CYS:HA   | 2.32                     | 0.59              |
| 1:E:677:SER:HB2  | 1:E:678:PRO:HD2  | 1.85                     | 0.59              |
| 1:E:752:GLY:O    | 1:E:756:LEU:HB2  | 2.01                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:253:MSE:HE1  | 1:F:313:HIS:ND1  | 2.17                     | 0.59              |
| 1:F:519:THR:HB   | 1:F:608:ALA:HA   | 1.83                     | 0.59              |
| 1:A:485:GLN:CG   | 1:A:488:TYR:H    | 2.16                     | 0.59              |
| 1:B:402:ALA:HB2  | 1:B:457:ILE:HD12 | 1.84                     | 0.59              |
| 1:C:223:GLY:HA2  | 1:C:362:ILE:HD12 | 1.85                     | 0.59              |
| 1:D:121:ASN:HD22 | 1:D:123:ARG:H    | 1.49                     | 0.59              |
| 1:F:181:CYS:SG   | 1:F:183:VAL:HG13 | 2.43                     | 0.59              |
| 1:F:213:GLY:CA   | 1:F:235:VAL:HG11 | 2.33                     | 0.59              |
| 1:A:270:GLU:N    | 1:A:378:ARG:HH12 | 2.01                     | 0.59              |
| 1:A:210:ILE:HG21 | 1:A:325:TYR:HE1  | 1.67                     | 0.59              |
| 1:A:408:MSE:HG3  | 1:A:424:TYR:HE1  | 1.68                     | 0.59              |
| 1:B:111:ASP:O    | 1:B:114:ARG:HG2  | 2.02                     | 0.59              |
| 1:B:237:ALA:HA   | 1:B:295:ASN:HD21 | 1.68                     | 0.59              |
| 1:C:491:ILE:HG22 | 1:C:527:LEU:HD12 | 1.84                     | 0.59              |
| 1:C:583:GLU:HG3  | 1:C:592:PHE:CD1  | 2.37                     | 0.59              |
| 1:D:485:GLN:HE21 | 1:D:487:HIS:N    | 1.87                     | 0.59              |
| 1:D:565:TYR:HB3  | 1:D:569:GLU:CB   | 2.33                     | 0.59              |
| 1:E:399:ASN:O    | 1:E:454:ASP:HB2  | 2.02                     | 0.59              |
| 1:F:253:MSE:HE3  | 1:F:317:PHE:CE1  | 2.38                     | 0.59              |
| 1:A:447:ILE:O    | 1:A:448:LEU:HD23 | 2.02                     | 0.59              |
| 1:A:620:VAL:C    | 1:A:622:LEU:H    | 2.06                     | 0.59              |
| 1:C:247:GLN:OE1  | 1:C:637:LYS:HE3  | 2.01                     | 0.59              |
| 1:C:591:GLU:HG2  | 1:F:475:ASN:ND2  | 2.17                     | 0.59              |
| 1:C:9:GLN:O      | 1:C:71:ASP:HB3   | 2.03                     | 0.59              |
| 1:E:274:LEU:HB3  | 1:E:307:LEU:HD11 | 1.85                     | 0.59              |
| 1:A:371:ILE:HG13 | 1:A:380:VAL:HA   | 1.85                     | 0.58              |
| 1:A:405:ALA:H    | 1:A:749:VAL:HG11 | 1.68                     | 0.58              |
| 1:E:15:VAL:HG12  | 1:E:16:GLY:H     | 1.66                     | 0.58              |
| 1:A:140:ILE:HB   | 1:A:152:THR:CG2  | 2.33                     | 0.58              |
| 1:B:108:ILE:HD11 | 1:B:314:TYR:CE2  | 2.38                     | 0.58              |
| 1:B:232:ASN:HB3  | 1:B:235:VAL:CG2  | 2.31                     | 0.58              |
| 1:B:433:VAL:O    | 1:B:436:PHE:HB3  | 2.04                     | 0.58              |
| 1:C:312:THR:HA   | 1:C:315:ILE:HG22 | 1.84                     | 0.58              |
| 1:C:642:ALA:O    | 1:C:683:TYR:HB2  | 2.03                     | 0.58              |
| 1:D:18:ARG:HA    | 1:D:21:VAL:HG12  | 1.85                     | 0.58              |
| 1:D:11:ILE:CG1   | 1:D:68:ALA:HA    | 2.29                     | 0.58              |
| 1:D:724:MSE:O    | 1:D:728:VAL:HG23 | 2.03                     | 0.58              |
| 1:E:589:LYS:HG3  | 1:E:590:VAL:N    | 2.17                     | 0.58              |
| 1:F:498:LYS:HB2  | 1:F:500:LEU:HD23 | 1.85                     | 0.58              |
| 1:F:506:ILE:HG12 | 1:F:524:VAL:HG12 | 1.85                     | 0.58              |
| 1:A:407:LEU:HD23 | 1:A:427:ASN:ND2  | 2.19                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:615:LEU:HD12 | 1:A:638:LEU:HD23 | 1.85                     | 0.58              |
| 1:B:154:LYS:O    | 1:B:154:LYS:HD3  | 2.02                     | 0.58              |
| 1:B:220:GLY:H    | 1:B:224:ILE:HA   | 1.68                     | 0.58              |
| 1:B:298:PRO:O    | 1:B:300:LEU:HD12 | 2.03                     | 0.58              |
| 1:B:337:MSE:HG3  | 1:B:367:ASP:OD2  | 2.02                     | 0.58              |
| 1:B:34:VAL:HG12  | 1:B:87:TYR:HE1   | 1.67                     | 0.58              |
| 1:C:253:MSE:HG2  | 1:C:317:PHE:CE1  | 2.32                     | 0.58              |
| 1:C:106:ILE:HG23 | 1:C:277:TYR:HB2  | 1.83                     | 0.58              |
| 1:C:57:ILE:HG23  | 1:C:73:ILE:HD11  | 1.86                     | 0.58              |
| 1:D:370:VAL:HG22 | 1:D:382:ARG:HB2  | 1.85                     | 0.58              |
| 1:D:247:GLN:HE22 | 1:D:637:LYS:HE3  | 1.68                     | 0.58              |
| 1:D:65:PRO:HG2   | 1:D:68:ALA:CB    | 2.33                     | 0.58              |
| 1:D:331:ASN:HD22 | 1:D:337:MSE:CA   | 2.13                     | 0.58              |
| 1:E:412:GLY:HA2  | 1:E:420:TYR:O    | 2.02                     | 0.58              |
| 1:A:140:ILE:HB   | 1:A:152:THR:HG22 | 1.84                     | 0.58              |
| 1:A:183:VAL:HG23 | 1:A:184:CYS:H    | 1.68                     | 0.58              |
| 1:B:278:ARG:CG   | 1:B:280:PRO:HD3  | 2.33                     | 0.58              |
| 1:C:500:LEU:HD13 | 1:C:736:PHE:CZ   | 2.38                     | 0.58              |
| 1:D:216:VAL:HG23 | 1:D:354:TYR:O    | 2.03                     | 0.58              |
| 1:E:264:ALA:HB2  | 1:E:286:LYS:HA   | 1.86                     | 0.58              |
| 1:E:376:GLY:HA2  | 1:E:726:ARG:HH11 | 1.68                     | 0.58              |
| 1:F:15:VAL:HG11  | 1:F:67:LEU:O     | 2.03                     | 0.58              |
| 1:A:66:PRO:HG3   | 1:A:133:ASN:O    | 2.04                     | 0.58              |
| 1:A:369:SER:N    | 1:A:385:ARG:HB2  | 2.19                     | 0.58              |
| 1:A:543:LEU:H    | 1:A:543:LEU:HD23 | 1.67                     | 0.58              |
| 1:B:329:SER:HB2  | 1:B:331:ASN:HD21 | 1.69                     | 0.58              |
| 1:C:225:HIS:ND1  | 1:C:337:MSE:HE1  | 2.18                     | 0.58              |
| 1:E:398:TYR:HB2  | 1:E:454:ASP:OD2  | 2.04                     | 0.58              |
| 1:F:524:VAL:HG22 | 1:F:536:ALA:O    | 2.04                     | 0.58              |
| 1:F:570:LEU:O    | 1:F:574:ILE:HG12 | 2.04                     | 0.58              |
| 1:A:190:LEU:HD12 | 1:A:355:PHE:O    | 2.04                     | 0.58              |
| 1:A:601:LYS:HB2  | 1:A:603:ILE:HG13 | 1.86                     | 0.58              |
| 1:A:374:VAL:HG11 | 1:A:744:ARG:HH22 | 1.69                     | 0.58              |
| 1:A:759:LEU:HD21 | 1:A:764:TYR:HB2  | 1.85                     | 0.58              |
| 1:B:623:ASN:ND2  | 1:B:624:VAL:HG23 | 2.18                     | 0.58              |
| 1:B:729:VAL:HG11 | 1:B:735:ASN:HB3  | 1.85                     | 0.58              |
| 1:C:11:ILE:HG12  | 1:C:68:ALA:HA    | 1.86                     | 0.58              |
| 1:E:490:HIS:HE1  | 1:E:746:ASP:HA   | 1.68                     | 0.58              |
| 1:F:461:HIS:O    | 1:F:467:THR:HG21 | 2.02                     | 0.58              |
| 1:F:583:GLU:HG3  | 1:F:592:PHE:CG   | 2.38                     | 0.58              |
| 1:F:580:LYS:HG3  | 1:F:593:ASN:ND2  | 2.17                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:434:LEU:HD13 | 1:A:465:ASN:HB3  | 1.85                     | 0.58              |
| 1:B:269:GLU:HB2  | 1:B:378:ARG:CZ   | 2.34                     | 0.58              |
| 1:B:628:ARG:HD2  | 1:B:634:PRO:CD   | 2.34                     | 0.58              |
| 1:C:216:VAL:HB   | 1:C:354:TYR:HB2  | 1.86                     | 0.58              |
| 1:C:620:VAL:C    | 1:C:622:LEU:H    | 2.04                     | 0.58              |
| 1:E:472:GLU:O    | 1:E:476:GLU:HG2  | 2.03                     | 0.58              |
| 1:E:487:HIS:CD2  | 1:E:520:TRP:HB3  | 2.39                     | 0.58              |
| 1:F:207:ALA:O    | 1:F:210:ILE:HG22 | 2.04                     | 0.58              |
| 1:B:189:ARG:HB3  | 1:B:191:TYR:CE2  | 2.39                     | 0.58              |
| 1:B:215:ILE:CD1  | 1:B:352:ALA:HA   | 2.33                     | 0.58              |
| 1:B:554:LEU:O    | 1:B:558:MSE:HG3  | 2.03                     | 0.58              |
| 1:D:225:HIS:HB2  | 1:D:328:THR:O    | 2.03                     | 0.58              |
| 1:F:760:TYR:CE2  | 1:F:767:LYS:HG2  | 2.39                     | 0.58              |
| 1:A:371:ILE:CB   | 1:A:380:VAL:HG13 | 2.33                     | 0.58              |
| 1:A:461:HIS:HE1  | 1:A:463:ALA:HB3  | 1.67                     | 0.58              |
| 1:C:218:ILE:O    | 1:C:224:ILE:HG13 | 2.04                     | 0.58              |
| 1:C:264:ALA:HB1  | 1:C:285:ARG:O    | 2.03                     | 0.58              |
| 1:D:572:GLY:HA2  | 1:D:575:ASN:ND2  | 2.19                     | 0.58              |
| 1:E:19:PRO:O     | 1:E:23:ARG:HG3   | 2.03                     | 0.58              |
| 1:E:401:LEU:HD12 | 1:E:402:ALA:H    | 1.69                     | 0.58              |
| 1:F:284:LEU:O    | 1:F:302:THR:HA   | 2.03                     | 0.58              |
| 1:F:281:ILE:HG12 | 1:F:306:MSE:CG   | 2.33                     | 0.58              |
| 1:A:226:LEU:HD21 | 1:A:351:VAL:HG12 | 1.86                     | 0.57              |
| 1:A:156:PHE:HZ   | 1:A:359:ASN:HB2  | 1.69                     | 0.57              |
| 1:A:433:VAL:O    | 1:A:436:PHE:HB3  | 2.04                     | 0.57              |
| 1:E:485:GLN:HG3  | 1:E:488:TYR:H    | 1.69                     | 0.57              |
| 1:A:215:ILE:O    | 1:A:353:ASP:HB2  | 2.04                     | 0.57              |
| 1:A:443:HIS:O    | 1:A:447:ILE:HD12 | 2.04                     | 0.57              |
| 1:A:582:VAL:CG1  | 1:A:626:TYR:HB3  | 2.34                     | 0.57              |
| 1:B:23:ARG:O     | 1:B:27:GLU:HB2   | 2.04                     | 0.57              |
| 1:E:127:PRO:O    | 1:E:311:GLY:HA3  | 2.04                     | 0.57              |
| 1:E:189:ARG:HD2  | 1:E:191:TYR:OH   | 2.04                     | 0.57              |
| 1:E:265:TYR:O    | 1:E:284:LEU:HD13 | 2.04                     | 0.57              |
| 1:F:620:VAL:C    | 1:F:622:LEU:H    | 2.06                     | 0.57              |
| 1:B:19:PRO:O     | 1:B:23:ARG:HG3   | 2.04                     | 0.57              |
| 1:B:283:THR:HA   | 1:B:303:ILE:O    | 2.04                     | 0.57              |
| 1:C:373:PHE:CE1  | 1:C:378:ARG:HB3  | 2.39                     | 0.57              |
| 1:C:590:VAL:N    | 1:F:475:ASN:HD21 | 2.02                     | 0.57              |
| 1:C:455:LEU:HD21 | 1:C:760:TYR:HE1  | 1.69                     | 0.57              |
| 1:E:700:ARG:HD2  | 1:E:704:PHE:HE2  | 1.68                     | 0.57              |
| 1:F:239:LEU:O    | 1:F:243:THR:HG22 | 2.02                     | 0.57              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:375:ASP:OD1  | 1:F:723:LYS:HE2  | 2.03                     | 0.57              |
| 1:F:729:VAL:O    | 1:F:729:VAL:HG12 | 2.05                     | 0.57              |
| 1:A:263:PHE:CZ   | 1:A:303:ILE:HG21 | 2.38                     | 0.57              |
| 1:B:270:GLU:OE1  | 1:B:284:LEU:HD21 | 2.04                     | 0.57              |
| 1:B:516:ASP:HB2  | 1:B:518:ASN:ND2  | 2.19                     | 0.57              |
| 1:B:557:LEU:O    | 1:B:557:LEU:HD23 | 2.03                     | 0.57              |
| 1:B:579:PRO:HB3  | 1:B:626:TYR:CE1  | 2.39                     | 0.57              |
| 1:B:504:ILE:HB   | 1:B:709:VAL:HG12 | 1.84                     | 0.57              |
| 1:D:560:ILE:HD12 | 1:D:561:LEU:N    | 2.18                     | 0.57              |
| 1:E:264:ALA:CB   | 1:E:286:LYS:HA   | 2.35                     | 0.57              |
| 1:E:394:ILE:HG22 | 1:E:396:PHE:H    | 1.69                     | 0.57              |
| 1:E:616:ASP:HB3  | 1:E:634:PRO:HG3  | 1.86                     | 0.57              |
| 1:F:171:ASN:ND2  | 1:F:173:ARG:HB2  | 2.20                     | 0.57              |
| 1:F:278:ARG:HG3  | 1:F:280:PRO:HD3  | 1.86                     | 0.57              |
| 1:F:708:ASN:N    | 1:F:708:ASN:ND2  | 2.51                     | 0.57              |
| 1:A:183:VAL:CG2  | 1:A:184:CYS:H    | 2.17                     | 0.57              |
| 1:A:580:LYS:NZ   | 1:A:590:VAL:HG22 | 2.20                     | 0.57              |
| 1:B:151:THR:HG23 | 1:B:153:MSE:H    | 1.69                     | 0.57              |
| 1:B:541:TYR:CG   | 1:B:560:ILE:HG22 | 2.39                     | 0.57              |
| 1:B:572:GLY:HA2  | 1:B:575:ASN:HD22 | 1.69                     | 0.57              |
| 1:C:183:VAL:HG23 | 1:C:184:CYS:N    | 2.19                     | 0.57              |
| 1:C:273:GLU:HG3  | 1:C:273:GLU:O    | 2.04                     | 0.57              |
| 1:D:197:GLU:O    | 1:D:198:ILE:HD13 | 2.05                     | 0.57              |
| 1:E:653:VAL:HG13 | 1:E:692:ALA:HB3  | 1.86                     | 0.57              |
| 1:A:193:SER:O    | 1:A:194:ASP:HB2  | 2.05                     | 0.57              |
| 1:A:603:ILE:HG23 | 1:B:516:ASP:HA   | 1.87                     | 0.57              |
| 1:B:37:LEU:O     | 1:B:37:LEU:HD13  | 2.04                     | 0.57              |
| 1:B:457:ILE:HG22 | 1:B:458:ALA:N    | 2.20                     | 0.57              |
| 1:C:171:ASN:ND2  | 1:C:173:ARG:H    | 2.02                     | 0.57              |
| 1:C:203:LEU:HD21 | 1:C:315:ILE:HD13 | 1.87                     | 0.57              |
| 1:C:690:ALA:CB   | 1:C:721:ILE:HG23 | 2.33                     | 0.57              |
| 1:C:88:ILE:HG22  | 1:C:89:GLU:N     | 2.19                     | 0.57              |
| 1:F:67:LEU:HD13  | 1:F:106:ILE:HD13 | 1.86                     | 0.57              |
| 1:F:383:ARG:HD2  | 1:F:387:PHE:CD2  | 2.40                     | 0.57              |
| 1:A:217:ALA:O    | 1:A:218:ILE:HD13 | 2.03                     | 0.57              |
| 1:A:30:LEU:HD11  | 1:A:53:ILE:HA    | 1.86                     | 0.57              |
| 1:A:401:LEU:HD12 | 1:A:402:ALA:H    | 1.70                     | 0.57              |
| 1:B:282:ILE:HD12 | 1:B:371:ILE:CG2  | 2.35                     | 0.57              |
| 1:D:21:VAL:HG11  | 1:D:34:VAL:HG21  | 1.87                     | 0.57              |
| 1:E:760:TYR:CE2  | 1:E:767:LYS:HG2  | 2.40                     | 0.57              |
| 1:A:219:LYS:HA   | 1:A:224:ILE:CG2  | 2.35                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:369:SER:HB2  | 1:B:385:ARG:HB3  | 1.86                     | 0.57              |
| 1:C:21:VAL:HG11  | 1:C:34:VAL:HG21  | 1.87                     | 0.57              |
| 1:D:633:GLU:N    | 1:D:634:PRO:HD2  | 2.19                     | 0.57              |
| 1:D:670:LEU:HA   | 1:D:673:ILE:HG12 | 1.86                     | 0.57              |
| 1:D:700:ARG:HD2  | 1:D:704:PHE:HE2  | 1.70                     | 0.57              |
| 1:E:52:ASP:O     | 1:E:56:PHE:HB2   | 2.04                     | 0.57              |
| 1:F:215:ILE:HG22 | 1:F:228:CYS:CB   | 2.35                     | 0.57              |
| 1:F:395:PRO:HG2  | 1:F:396:PHE:CE2  | 2.40                     | 0.57              |
| 1:B:677:SER:HB2  | 1:B:678:PRO:HD2  | 1.86                     | 0.57              |
| 1:C:169:PRO:HA   | 1:C:174:TYR:CD2  | 2.40                     | 0.57              |
| 1:C:201:ASP:N    | 1:C:202:PRO:CD   | 2.66                     | 0.57              |
| 1:C:21:VAL:HA    | 1:C:24:ILE:HG22  | 1.87                     | 0.57              |
| 1:D:200:GLY:C    | 1:D:202:PRO:HD2  | 2.25                     | 0.57              |
| 1:E:171:ASN:ND2  | 1:E:173:ARG:HB2  | 2.19                     | 0.57              |
| 1:F:218:ILE:HD12 | 1:F:356:LEU:HD23 | 1.87                     | 0.57              |
| 1:F:498:LYS:CB   | 1:F:500:LEU:HD23 | 2.35                     | 0.57              |
| 1:A:202:PRO:O    | 1:A:203:LEU:C    | 2.43                     | 0.57              |
| 1:A:384:SER:HA   | 1:A:388:VAL:HG23 | 1.86                     | 0.57              |
| 1:B:268:PRO:C    | 1:B:270:GLU:H    | 2.09                     | 0.57              |
| 1:B:35:LYS:HE2   | 1:B:90:LYS:HD2   | 1.87                     | 0.57              |
| 1:B:497:GLU:OE2  | 1:B:741:GLU:HB3  | 2.05                     | 0.57              |
| 1:B:759:LEU:CD1  | 1:B:764:TYR:HB2  | 2.35                     | 0.57              |
| 1:C:504:ILE:HG22 | 1:C:505:GLY:N    | 2.19                     | 0.57              |
| 1:E:288:GLU:CB   | 1:E:289:PRO:HD3  | 2.31                     | 0.57              |
| 1:E:494:VAL:C    | 1:E:496:ALA:H    | 2.08                     | 0.57              |
| 1:F:15:VAL:HG12  | 1:F:16:GLY:N     | 2.19                     | 0.57              |
| 1:F:371:ILE:CD1  | 1:F:380:VAL:HG22 | 2.33                     | 0.57              |
| 1:F:494:VAL:HG22 | 1:F:738:VAL:HG22 | 1.86                     | 0.57              |
| 1:A:502:SER:O    | 1:A:503:VAL:HG13 | 2.05                     | 0.56              |
| 1:A:24:ILE:HG23  | 1:A:56:PHE:CE1   | 2.40                     | 0.56              |
| 1:B:127:PRO:HB3  | 1:B:312:THR:HG22 | 1.87                     | 0.56              |
| 1:B:19:PRO:HG3   | 1:B:174:TYR:HD1  | 1.69                     | 0.56              |
| 1:C:105:ASP:CG   | 1:C:139:THR:HG23 | 2.25                     | 0.56              |
| 1:C:127:PRO:HB3  | 1:C:312:THR:CG2  | 2.28                     | 0.56              |
| 1:D:111:ASP:HB3  | 1:D:172:ARG:NH1  | 2.14                     | 0.56              |
| 1:D:760:TYR:HE2  | 1:D:767:LYS:HG2  | 1.70                     | 0.56              |
| 1:E:189:ARG:HB3  | 1:E:191:TYR:CE2  | 2.40                     | 0.56              |
| 1:E:457:ILE:HG22 | 1:E:458:ALA:H    | 1.70                     | 0.56              |
| 1:A:102:ILE:CD1  | 1:A:144:LEU:HG   | 2.34                     | 0.56              |
| 1:A:144:LEU:HD23 | 1:A:146:TYR:H    | 1.69                     | 0.56              |
| 1:A:171:ASN:HD21 | 1:A:173:ARG:HB2  | 1.70                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:269:GLU:HB2  | 1:A:378:ARG:CZ   | 2.35                     | 0.56              |
| 1:A:335:MSE:CE   | 1:A:430:LYS:HG3  | 2.32                     | 0.56              |
| 1:A:759:LEU:O    | 1:A:762:GLU:HB2  | 2.04                     | 0.56              |
| 1:C:408:MSE:HG3  | 1:C:424:TYR:CE1  | 2.40                     | 0.56              |
| 1:C:654:PRO:HG2  | 1:C:661:ARG:HB2  | 1.88                     | 0.56              |
| 1:D:380:VAL:HG21 | 1:D:740:THR:HG23 | 1.87                     | 0.56              |
| 1:D:495:MSE:HE2  | 1:D:755:PHE:HZ   | 1.68                     | 0.56              |
| 1:E:122:LYS:HE3  | 1:E:161:PHE:CZ   | 2.39                     | 0.56              |
| 1:E:331:ASN:ND2  | 1:E:337:MSE:HA   | 2.17                     | 0.56              |
| 1:F:140:ILE:HB   | 1:F:152:THR:HG22 | 1.87                     | 0.56              |
| 1:F:192:THR:C    | 1:F:194:ASP:H    | 2.08                     | 0.56              |
| 1:F:301:HIS:CD2  | 1:F:302:THR:H    | 2.22                     | 0.56              |
| 1:F:582:VAL:HG13 | 1:F:627:ARG:HG2  | 1.88                     | 0.56              |
| 1:A:5:HIS:CE1    | 1:A:43:GLU:HG2   | 2.40                     | 0.56              |
| 1:A:612:GLY:O    | 1:A:616:ASP:HB2  | 2.06                     | 0.56              |
| 1:E:306:MSE:HE1  | 1:E:309:TYR:HE2  | 1.70                     | 0.56              |
| 1:E:408:MSE:HG3  | 1:E:424:TYR:HE1  | 1.69                     | 0.56              |
| 1:A:398:TYR:HB2  | 1:A:454:ASP:OD2  | 2.05                     | 0.56              |
| 1:B:689:LEU:O    | 1:B:693:PHE:HB2  | 2.04                     | 0.56              |
| 1:C:286:LYS:HE3  | 1:C:290:PHE:HA   | 1.88                     | 0.56              |
| 1:D:567:ILE:HG12 | 1:D:600:ALA:HB1  | 1.85                     | 0.56              |
| 1:D:665:LEU:O    | 1:D:669:ILE:HG13 | 2.05                     | 0.56              |
| 1:E:737:HIS:O    | 1:E:738:VAL:C    | 2.44                     | 0.56              |
| 1:F:381:ILE:HG22 | 1:F:717:TYR:CE1  | 2.40                     | 0.56              |
| 1:F:488:TYR:O    | 1:F:492:ALA:HB2  | 2.04                     | 0.56              |
| 1:A:136:PRO:HG3  | 1:A:360:ARG:NH1  | 2.21                     | 0.56              |
| 1:B:296:LEU:HD12 | 1:B:296:LEU:H    | 1.70                     | 0.56              |
| 1:B:398:TYR:HB2  | 1:B:454:ASP:CG   | 2.26                     | 0.56              |
| 1:C:126:TYR:CD1  | 1:C:182:PRO:HG3  | 2.40                     | 0.56              |
| 1:C:18:ARG:HH21  | 1:C:36:ASN:HD22  | 1.53                     | 0.56              |
| 1:C:683:TYR:CZ   | 1:C:687:LEU:HD11 | 2.40                     | 0.56              |
| 1:D:756:LEU:O    | 1:D:759:LEU:HB3  | 2.05                     | 0.56              |
| 1:E:341:ASN:O    | 1:E:344:ALA:HB3  | 2.05                     | 0.56              |
| 1:E:365:ARG:O    | 1:E:423:GLN:HG2  | 2.06                     | 0.56              |
| 1:E:756:LEU:O    | 1:E:759:LEU:HB3  | 2.05                     | 0.56              |
| 1:A:137:ARG:O    | 1:A:141:ILE:HG13 | 2.06                     | 0.56              |
| 1:A:153:MSE:HE1  | 1:A:360:ARG:HD3  | 1.86                     | 0.56              |
| 1:A:552:TYR:CZ   | 1:A:627:ARG:HD2  | 2.41                     | 0.56              |
| 1:B:504:ILE:O    | 1:B:709:VAL:HA   | 2.06                     | 0.56              |
| 1:C:137:ARG:O    | 1:C:141:ILE:HG13 | 2.05                     | 0.56              |
| 1:D:616:ASP:O    | 1:D:620:VAL:HG23 | 2.05                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:224:ILE:CG1  | 1:E:338:VAL:HG13 | 2.36                     | 0.56              |
| 1:E:215:ILE:HG12 | 1:E:353:ASP:OD2  | 2.04                     | 0.56              |
| 1:E:633:GLU:N    | 1:E:634:PRO:CD   | 2.69                     | 0.56              |
| 1:E:690:ALA:HB2  | 1:E:721:ILE:HG23 | 1.86                     | 0.56              |
| 1:E:379:ALA:HB3  | 1:E:744:ARG:NH1  | 2.20                     | 0.56              |
| 1:F:104:PRO:HD3  | 1:F:390:LEU:HD21 | 1.86                     | 0.56              |
| 1:F:497:GLU:OE2  | 1:F:741:GLU:HB3  | 2.06                     | 0.56              |
| 1:A:281:ILE:HG12 | 1:A:306:MSE:CG   | 2.32                     | 0.56              |
| 1:A:108:ILE:CG1  | 1:A:311:GLY:H    | 2.18                     | 0.56              |
| 1:A:522:GLY:HA3  | 1:A:611:THR:HG23 | 1.87                     | 0.56              |
| 1:B:148:ARG:CZ   | 1:B:158:MSE:HG3  | 2.35                     | 0.56              |
| 1:B:215:ILE:HG12 | 1:B:353:ASP:OD2  | 2.05                     | 0.56              |
| 1:B:678:PRO:HG2  | 1:B:679:ALA:H    | 1.71                     | 0.56              |
| 1:C:545:GLY:HA3  | 1:C:548:LEU:HD12 | 1.88                     | 0.56              |
| 1:D:561:LEU:HB2  | 1:D:570:LEU:HD11 | 1.88                     | 0.56              |
| 1:E:181:CYS:SG   | 1:E:182:PRO:N    | 2.79                     | 0.56              |
| 1:E:34:VAL:HB    | 1:E:87:TYR:OH    | 2.04                     | 0.56              |
| 1:F:461:HIS:CE1  | 1:F:463:ALA:HB3  | 2.40                     | 0.56              |
| 1:F:653:VAL:HG13 | 1:F:692:ALA:CB   | 2.30                     | 0.56              |
| 1:A:487:HIS:CE1  | 1:A:512:GLY:HA3  | 2.40                     | 0.56              |
| 1:B:464:TYR:HB2  | 1:B:467:THR:HG23 | 1.86                     | 0.56              |
| 1:C:310:ALA:O    | 1:C:313:HIS:HB2  | 2.06                     | 0.56              |
| 1:C:629:HIS:HB2  | 1:C:633:GLU:OE1  | 2.06                     | 0.56              |
| 1:D:330:ALA:O    | 1:D:338:VAL:HG12 | 2.05                     | 0.56              |
| 1:D:339:LYS:HG3  | 1:D:365:ARG:NH1  | 2.21                     | 0.56              |
| 1:D:401:LEU:HD12 | 1:D:402:ALA:H    | 1.71                     | 0.56              |
| 1:F:500:LEU:HD13 | 1:F:503:VAL:HG11 | 1.87                     | 0.56              |
| 1:A:236:VAL:CG1  | 1:A:295:ASN:HD22 | 2.18                     | 0.56              |
| 1:A:540:TYR:HD1  | 1:A:540:TYR:H    | 1.53                     | 0.56              |
| 1:B:261:LYS:HE2  | 1:B:266:VAL:HG21 | 1.88                     | 0.56              |
| 1:B:498:LYS:HB2  | 1:B:500:LEU:HD23 | 1.88                     | 0.56              |
| 1:B:655:VAL:HG22 | 1:B:660:ILE:HG23 | 1.88                     | 0.56              |
| 1:C:457:ILE:CG2  | 1:C:753:GLN:HB3  | 2.34                     | 0.56              |
| 1:D:228:CYS:SG   | 1:D:229:ASP:N    | 2.79                     | 0.56              |
| 1:D:331:ASN:ND2  | 1:D:337:MSE:HA   | 2.13                     | 0.56              |
| 1:E:558:MSE:HE1  | 1:E:593:ASN:OD1  | 2.06                     | 0.56              |
| 1:F:344:ALA:HA   | 1:F:348:LEU:HD13 | 1.87                     | 0.56              |
| 1:F:409:ASN:O    | 1:F:425:ILE:HG12 | 2.06                     | 0.56              |
| 1:A:226:LEU:HD11 | 1:A:348:LEU:HD23 | 1.87                     | 0.56              |
| 1:A:491:ILE:HG12 | 1:A:527:LEU:HD12 | 1.87                     | 0.56              |
| 1:B:171:ASN:HD21 | 1:B:173:ARG:HB2  | 1.71                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:627:ARG:HB2  | 1:B:629:HIS:CE1  | 2.41                     | 0.56              |
| 1:C:286:LYS:HZ2  | 1:C:291:PRO:HD2  | 1.71                     | 0.56              |
| 1:E:678:PRO:HG2  | 1:E:679:ALA:H    | 1.71                     | 0.56              |
| 1:E:708:ASN:HB3  | 1:E:734:LEU:O    | 2.05                     | 0.56              |
| 1:F:123:ARG:HH22 | 1:F:173:ARG:HG2  | 1.71                     | 0.56              |
| 1:F:756:LEU:HD21 | 1:F:770:LEU:CD2  | 2.36                     | 0.56              |
| 1:A:189:ARG:O    | 1:A:356:LEU:HD12 | 2.06                     | 0.56              |
| 1:A:37:LEU:HB3   | 1:A:41:GLY:HA3   | 1.88                     | 0.56              |
| 1:B:413:VAL:HG21 | 1:B:448:LEU:HD13 | 1.86                     | 0.56              |
| 1:B:503:VAL:O    | 1:B:527:LEU:HD12 | 2.06                     | 0.56              |
| 1:B:485:GLN:OE1  | 1:B:514:GLY:HA2  | 2.06                     | 0.56              |
| 1:C:282:ILE:HG22 | 1:C:305:VAL:HB   | 1.88                     | 0.56              |
| 1:C:524:VAL:HG23 | 1:C:535:LEU:HB2  | 1.88                     | 0.56              |
| 1:C:650:LYS:HD2  | 1:C:691:ARG:NH2  | 2.21                     | 0.56              |
| 1:C:379:ALA:HB3  | 1:C:744:ARG:NH1  | 2.21                     | 0.56              |
| 1:D:504:ILE:HD12 | 1:D:701:ALA:HA   | 1.88                     | 0.56              |
| 1:A:364:ASN:HD21 | 1:A:443:HIS:CD2  | 2.24                     | 0.55              |
| 1:B:434:LEU:HD13 | 1:B:465:ASN:HB3  | 1.87                     | 0.55              |
| 1:B:524:VAL:HG23 | 1:B:535:LEU:HB2  | 1.88                     | 0.55              |
| 1:C:102:ILE:HD11 | 1:C:144:LEU:HG   | 1.88                     | 0.55              |
| 1:C:219:LYS:NZ   | 1:C:362:ILE:HG12 | 2.20                     | 0.55              |
| 1:C:269:GLU:O    | 1:C:272:GLU:HB3  | 2.06                     | 0.55              |
| 1:C:516:ASP:HB2  | 1:C:518:ASN:ND2  | 2.21                     | 0.55              |
| 1:C:582:VAL:HG11 | 1:C:626:TYR:O    | 2.05                     | 0.55              |
| 1:D:312:THR:HA   | 1:D:315:ILE:HG22 | 1.89                     | 0.55              |
| 1:E:700:ARG:HD2  | 1:E:704:PHE:CE2  | 2.41                     | 0.55              |
| 1:A:371:ILE:CD1  | 1:A:380:VAL:HG22 | 2.35                     | 0.55              |
| 1:A:456:ILE:CG2  | 1:A:457:ILE:H    | 2.16                     | 0.55              |
| 1:A:247:GLN:NE2  | 1:A:637:LYS:HE3  | 2.20                     | 0.55              |
| 1:C:225:HIS:NE2  | 1:C:327:MSE:HE3  | 2.21                     | 0.55              |
| 1:C:525:LEU:HD23 | 1:C:534:ARG:HA   | 1.88                     | 0.55              |
| 1:C:561:LEU:HB2  | 1:C:570:LEU:HD11 | 1.88                     | 0.55              |
| 1:C:628:ARG:NH2  | 1:C:632:GLY:H    | 2.03                     | 0.55              |
| 1:C:665:LEU:O    | 1:C:669:ILE:HG13 | 2.07                     | 0.55              |
| 1:D:370:VAL:HG23 | 1:D:381:ILE:CG1  | 2.37                     | 0.55              |
| 1:D:506:ILE:HB   | 1:D:711:LEU:HD12 | 1.87                     | 0.55              |
| 1:E:380:VAL:HG12 | 1:E:382:ARG:H    | 1.71                     | 0.55              |
| 1:E:401:LEU:O    | 1:E:456:ILE:HA   | 2.07                     | 0.55              |
| 1:E:610:SER:O    | 1:E:614:VAL:HG23 | 2.07                     | 0.55              |
| 1:F:53:ILE:HG23  | 1:F:54:GLU:HG3   | 1.89                     | 0.55              |
| 1:A:190:LEU:HD13 | 1:A:356:LEU:HD13 | 1.88                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:580:LYS:HG2  | 1:B:593:ASN:HD22 | 1.71                     | 0.55              |
| 1:B:587:TYR:HD1  | 1:B:588:GLY:N    | 2.00                     | 0.55              |
| 1:C:339:LYS:HG3  | 1:C:365:ARG:HH12 | 1.70                     | 0.55              |
| 1:C:554:LEU:HG   | 1:C:558:MSE:HE3  | 1.88                     | 0.55              |
| 1:C:522:GLY:CA   | 1:C:611:THR:HG23 | 2.36                     | 0.55              |
| 1:D:282:ILE:HA   | 1:D:371:ILE:O    | 2.06                     | 0.55              |
| 1:D:624:VAL:HG12 | 1:D:637:LYS:HD3  | 1.87                     | 0.55              |
| 1:E:338:VAL:HG21 | 1:E:344:ALA:HA   | 1.88                     | 0.55              |
| 1:F:218:ILE:C    | 1:F:224:ILE:HG23 | 2.27                     | 0.55              |
| 1:F:737:HIS:O    | 1:F:738:VAL:C    | 2.44                     | 0.55              |
| 1:F:22:TYR:CE1   | 1:F:87:TYR:HB3   | 2.40                     | 0.55              |
| 1:B:527:LEU:HD12 | 1:B:527:LEU:H    | 1.72                     | 0.55              |
| 1:C:102:ILE:HG23 | 1:C:141:ILE:CD1  | 2.37                     | 0.55              |
| 1:C:268:PRO:HG2  | 1:C:269:GLU:OE1  | 2.06                     | 0.55              |
| 1:E:225:HIS:HA   | 1:E:330:ALA:CB   | 2.37                     | 0.55              |
| 1:E:582:VAL:HG13 | 1:E:626:TYR:HB3  | 1.88                     | 0.55              |
| 1:F:286:LYS:HB2  | 1:F:303:ILE:HD12 | 1.87                     | 0.55              |
| 1:F:253:MSE:O    | 1:F:317:PHE:HZ   | 1.89                     | 0.55              |
| 1:F:397:GLU:HB2  | 1:F:416:ASN:HA   | 1.88                     | 0.55              |
| 1:C:219:LYS:HA   | 1:C:224:ILE:CB   | 2.35                     | 0.55              |
| 1:C:601:LYS:HD3  | 1:F:772:LEU:HD11 | 1.87                     | 0.55              |
| 1:E:196:GLN:HG2  | 1:E:197:GLU:O    | 2.07                     | 0.55              |
| 1:F:8:VAL:HG12   | 1:F:12:VAL:HG11  | 1.88                     | 0.55              |
| 1:F:580:LYS:HZ1  | 1:F:590:VAL:HG22 | 1.71                     | 0.55              |
| 1:A:498:LYS:HE3  | 1:A:736:PHE:HB2  | 1.89                     | 0.55              |
| 1:B:123:ARG:HH22 | 1:B:173:ARG:HG2  | 1.72                     | 0.55              |
| 1:B:294:GLU:HG2  | 1:B:294:GLU:O    | 2.07                     | 0.55              |
| 1:B:3:ALA:HB2    | 1:B:47:GLU:HA    | 1.89                     | 0.55              |
| 1:C:196:GLN:HG2  | 1:C:197:GLU:O    | 2.07                     | 0.55              |
| 1:D:125:MSE:O    | 1:D:127:PRO:HD3  | 2.06                     | 0.55              |
| 1:D:24:ILE:HG12  | 1:D:56:PHE:HD1   | 1.72                     | 0.55              |
| 1:D:457:ILE:HG21 | 1:D:753:GLN:HB3  | 1.89                     | 0.55              |
| 1:D:522:GLY:HA2  | 1:D:611:THR:HG23 | 1.88                     | 0.55              |
| 1:F:14:ALA:HB3   | 1:F:103:PRO:CD   | 2.36                     | 0.55              |
| 1:F:406:GLU:HG3  | 1:F:407:LEU:HG   | 1.89                     | 0.55              |
| 1:A:216:VAL:HG23 | 1:A:354:TYR:C    | 2.27                     | 0.55              |
| 1:A:572:GLY:O    | 1:A:575:ASN:HB2  | 2.07                     | 0.55              |
| 1:A:580:LYS:HZ2  | 1:A:590:VAL:HG13 | 1.71                     | 0.55              |
| 1:B:142:GLU:O    | 1:B:143:ASP:HB3  | 2.07                     | 0.55              |
| 1:B:491:ILE:CG2  | 1:B:527:LEU:HD11 | 2.36                     | 0.55              |
| 1:C:123:ARG:NH2  | 1:C:173:ARG:HE   | 2.05                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:128:PHE:CD1  | 1:E:186:PRO:HG2  | 2.41                     | 0.55              |
| 1:E:330:ALA:O    | 1:E:338:VAL:HG12 | 2.07                     | 0.55              |
| 1:E:515:THR:O    | 1:E:516:ASP:HB2  | 2.05                     | 0.55              |
| 1:F:193:SER:O    | 1:F:194:ASP:CB   | 2.54                     | 0.55              |
| 1:F:399:ASN:HA   | 1:F:414:ALA:O    | 2.06                     | 0.55              |
| 1:F:665:LEU:HG   | 1:F:669:ILE:HD11 | 1.88                     | 0.55              |
| 1:A:193:SER:O    | 1:A:194:ASP:CB   | 2.54                     | 0.55              |
| 1:A:408:MSE:HG3  | 1:A:424:TYR:CE1  | 2.41                     | 0.55              |
| 1:A:522:GLY:CA   | 1:A:611:THR:HG23 | 2.37                     | 0.55              |
| 1:A:742:VAL:HG11 | 1:A:751:VAL:HG11 | 1.88                     | 0.55              |
| 1:B:11:ILE:O     | 1:B:11:ILE:HG23  | 2.07                     | 0.55              |
| 1:B:664:GLU:O    | 1:B:667:GLN:HB3  | 2.07                     | 0.55              |
| 1:B:738:VAL:HB   | 1:B:744:ARG:HG3  | 1.87                     | 0.55              |
| 1:B:749:VAL:O    | 1:B:753:GLN:HG3  | 2.06                     | 0.55              |
| 1:C:249:PRO:HG3  | 1:C:300:LEU:CD1  | 2.37                     | 0.55              |
| 1:A:727:LYS:HZ1  | 1:C:287:LYS:HE3  | 1.71                     | 0.55              |
| 1:C:670:LEU:HA   | 1:C:673:ILE:HG12 | 1.89                     | 0.55              |
| 1:C:15:VAL:HG21  | 1:C:67:LEU:O     | 2.06                     | 0.55              |
| 1:D:57:ILE:HG13  | 1:D:75:LYS:NZ    | 2.22                     | 0.55              |
| 1:E:562:SER:HB3  | 1:E:599:LEU:HD11 | 1.88                     | 0.55              |
| 1:E:582:VAL:HG11 | 1:E:626:TYR:O    | 2.06                     | 0.55              |
| 1:E:508:LEU:CD2  | 1:E:611:THR:HG21 | 2.37                     | 0.55              |
| 1:E:649:LEU:HB3  | 1:E:684:SER:CB   | 2.36                     | 0.55              |
| 1:F:494:VAL:HG11 | 1:F:710:ALA:HB1  | 1.88                     | 0.55              |
| 1:F:501:ASP:O    | 1:F:503:VAL:HG13 | 2.07                     | 0.55              |
| 1:B:252:ILE:HG23 | 1:B:325:TYR:O    | 2.07                     | 0.55              |
| 1:B:707:LYS:HG3  | 1:B:708:ASN:ND2  | 2.22                     | 0.55              |
| 1:C:500:LEU:HD13 | 1:C:736:PHE:CE2  | 2.42                     | 0.55              |
| 1:D:401:LEU:HD12 | 1:D:402:ALA:N    | 2.22                     | 0.55              |
| 1:E:147:ASP:HA   | 1:E:177:GLU:OE2  | 2.07                     | 0.55              |
| 1:A:651:PHE:HB2  | 1:A:688:ALA:CB   | 2.36                     | 0.55              |
| 1:B:224:ILE:HG12 | 1:B:338:VAL:O    | 2.06                     | 0.55              |
| 1:B:398:TYR:HB2  | 1:B:454:ASP:OD2  | 2.07                     | 0.55              |
| 1:B:525:LEU:HA   | 1:B:535:LEU:HD13 | 1.88                     | 0.55              |
| 1:B:53:ILE:O     | 1:B:57:ILE:HG12  | 2.07                     | 0.55              |
| 1:C:67:LEU:HD11  | 1:C:106:ILE:HD11 | 1.89                     | 0.55              |
| 1:C:142:GLU:HB2  | 1:C:150:ASN:O    | 2.07                     | 0.55              |
| 1:C:315:ILE:HG23 | 1:C:316:LEU:N    | 2.22                     | 0.55              |
| 1:C:369:SER:HB2  | 1:C:385:ARG:HB3  | 1.88                     | 0.55              |
| 1:D:119:PRO:HA   | 1:D:124:TYR:CD2  | 2.42                     | 0.55              |
| 1:D:737:HIS:O    | 1:D:738:VAL:C    | 2.46                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:538:ILE:HD11 | 1:E:611:THR:HG22 | 1.89                     | 0.55              |
| 1:F:20:PHE:HE1   | 1:F:60:LEU:HA    | 1.73                     | 0.55              |
| 1:F:545:GLY:HA3  | 1:F:548:LEU:HD12 | 1.89                     | 0.55              |
| 1:F:503:VAL:HG11 | 1:F:708:ASN:OD1  | 2.07                     | 0.55              |
| 1:A:245:ARG:NE   | 1:A:248:LYS:HB3  | 2.22                     | 0.54              |
| 1:A:282:ILE:HA   | 1:A:371:ILE:O    | 2.07                     | 0.54              |
| 1:A:724:MSE:O    | 1:A:728:VAL:HG23 | 2.07                     | 0.54              |
| 1:B:583:GLU:OE1  | 1:B:583:GLU:N    | 2.40                     | 0.54              |
| 1:C:114:ARG:O    | 1:C:118:ASP:HB2  | 2.07                     | 0.54              |
| 1:E:155:GLU:O    | 1:E:157:PRO:HD3  | 2.07                     | 0.54              |
| 1:F:237:ALA:HA   | 1:F:295:ASN:ND2  | 2.21                     | 0.54              |
| 1:F:239:LEU:HD22 | 1:F:250:PHE:CZ   | 2.42                     | 0.54              |
| 1:A:247:GLN:HE21 | 1:A:298:PRO:HG2  | 1.72                     | 0.54              |
| 1:B:124:TYR:CE2  | 1:B:125:MSE:HG2  | 2.42                     | 0.54              |
| 1:B:213:GLY:CA   | 1:B:235:VAL:HG11 | 2.36                     | 0.54              |
| 1:B:35:LYS:HG2   | 1:B:36:ASN:N     | 2.22                     | 0.54              |
| 1:B:528:GLY:O    | 1:B:529:TYR:C    | 2.45                     | 0.54              |
| 1:C:102:ILE:HD12 | 1:C:141:ILE:HG21 | 1.89                     | 0.54              |
| 1:D:140:ILE:HB   | 1:D:152:THR:CG2  | 2.38                     | 0.54              |
| 1:E:616:ASP:HA   | 1:E:634:PRO:HB2  | 1.90                     | 0.54              |
| 1:F:261:LYS:HZ3  | 1:F:266:VAL:HB   | 1.68                     | 0.54              |
| 1:F:265:TYR:CD2  | 1:F:265:TYR:N    | 2.75                     | 0.54              |
| 1:F:320:SER:O    | 1:F:321:LYS:C    | 2.46                     | 0.54              |
| 1:A:494:VAL:HG11 | 1:A:710:ALA:HB1  | 1.89                     | 0.54              |
| 1:C:586:LYS:CB   | 1:C:627:ARG:HH12 | 2.20                     | 0.54              |
| 1:D:315:ILE:HG12 | 1:D:319:TRP:CZ3  | 2.40                     | 0.54              |
| 1:D:593:ASN:O    | 1:D:596:LEU:HB2  | 2.08                     | 0.54              |
| 1:D:601:LYS:CB   | 1:D:603:ILE:HG13 | 2.38                     | 0.54              |
| 1:E:565:TYR:HB3  | 1:E:569:GLU:HB2  | 1.90                     | 0.54              |
| 1:F:190:LEU:HD21 | 1:F:206:ALA:CB   | 2.32                     | 0.54              |
| 1:F:506:ILE:HD11 | 1:F:697:ALA:HB2  | 1.88                     | 0.54              |
| 1:A:558:MSE:HB3  | 1:A:570:LEU:HD21 | 1.89                     | 0.54              |
| 1:A:649:LEU:HB3  | 1:A:684:SER:CB   | 2.37                     | 0.54              |
| 1:A:61:TYR:CZ    | 1:A:73:ILE:HD12  | 2.42                     | 0.54              |
| 1:C:227:ALA:HA   | 1:C:326:VAL:O    | 2.07                     | 0.54              |
| 1:C:553:PRO:HB2  | 1:C:620:VAL:HG21 | 1.87                     | 0.54              |
| 1:D:383:ARG:HG3  | 1:D:383:ARG:HH11 | 1.71                     | 0.54              |
| 1:D:655:VAL:HG22 | 1:D:660:ILE:HG12 | 1.89                     | 0.54              |
| 1:F:114:ARG:HG2  | 1:F:118:ASP:OD2  | 2.06                     | 0.54              |
| 1:F:232:ASN:HB3  | 1:F:235:VAL:HG22 | 1.88                     | 0.54              |
| 1:A:317:PHE:CE2  | 1:A:323:PRO:HA   | 2.42                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:35:LYS:HG2   | 1:A:36:ASN:H     | 1.72                     | 0.54              |
| 1:A:385:ARG:HG3  | 1:A:386:GLY:N    | 2.22                     | 0.54              |
| 1:B:484:VAL:HG12 | 1:B:770:LEU:HD13 | 1.89                     | 0.54              |
| 1:C:19:PRO:O     | 1:C:23:ARG:HG3   | 2.08                     | 0.54              |
| 1:C:370:VAL:HG23 | 1:C:381:ILE:HD11 | 1.88                     | 0.54              |
| 1:D:140:ILE:HB   | 1:D:152:THR:HG22 | 1.89                     | 0.54              |
| 1:D:628:ARG:CZ   | 1:D:632:GLY:H    | 2.20                     | 0.54              |
| 1:D:711:LEU:HD23 | 1:D:737:HIS:NE2  | 2.22                     | 0.54              |
| 1:E:273:GLU:HG2  | 1:E:371:ILE:HD13 | 1.88                     | 0.54              |
| 1:E:434:LEU:HD13 | 1:E:465:ASN:HB3  | 1.90                     | 0.54              |
| 1:F:215:ILE:HG21 | 1:F:239:LEU:HD12 | 1.90                     | 0.54              |
| 1:F:341:ASN:ND2  | 1:F:357:LEU:HB3  | 2.22                     | 0.54              |
| 1:F:391:PRO:HB3  | 1:F:420:TYR:CE1  | 2.42                     | 0.54              |
| 1:F:729:VAL:HB   | 1:F:735:ASN:ND2  | 2.23                     | 0.54              |
| 1:B:406:GLU:O    | 1:B:428:THR:HG23 | 2.07                     | 0.54              |
| 1:B:374:VAL:HG11 | 1:B:744:ARG:NH2  | 2.22                     | 0.54              |
| 1:C:738:VAL:CG2  | 1:C:744:ARG:HB3  | 2.37                     | 0.54              |
| 1:D:484:VAL:HG12 | 1:D:770:LEU:HD22 | 1.90                     | 0.54              |
| 1:E:50:GLU:O     | 1:E:53:ILE:HG22  | 2.08                     | 0.54              |
| 1:E:580:LYS:HG3  | 1:E:593:ASN:ND2  | 2.20                     | 0.54              |
| 1:F:369:SER:HB2  | 1:F:385:ARG:CB   | 2.37                     | 0.54              |
| 1:F:651:PHE:HB2  | 1:F:688:ALA:HB2  | 1.89                     | 0.54              |
| 1:F:739:THR:HG23 | 1:F:741:GLU:H    | 1.71                     | 0.54              |
| 1:A:370:VAL:HG23 | 1:A:381:ILE:HD11 | 1.88                     | 0.54              |
| 1:A:8:VAL:HA     | 1:A:72:ARG:O     | 2.08                     | 0.54              |
| 1:B:465:ASN:O    | 1:B:468:LYS:HB3  | 2.08                     | 0.54              |
| 1:B:682:ALA:O    | 1:B:686:HIS:HB2  | 2.07                     | 0.54              |
| 1:D:553:PRO:HB2  | 1:D:620:VAL:CG2  | 2.38                     | 0.54              |
| 1:E:339:LYS:HA   | 1:E:362:ILE:HD11 | 1.90                     | 0.54              |
| 1:E:504:ILE:O    | 1:E:709:VAL:HA   | 2.06                     | 0.54              |
| 1:F:495:MSE:HE2  | 1:F:755:PHE:CZ   | 2.42                     | 0.54              |
| 1:A:282:ILE:HD12 | 1:A:371:ILE:HG23 | 1.89                     | 0.54              |
| 1:B:183:VAL:HG23 | 1:B:184:CYS:N    | 2.23                     | 0.54              |
| 1:C:215:ILE:HD11 | 1:C:352:ALA:HA   | 1.89                     | 0.54              |
| 1:F:554:LEU:HD11 | 1:F:579:PRO:CB   | 2.36                     | 0.54              |
| 1:B:1:MSE:HE3    | 1:B:2:LYS:N      | 2.23                     | 0.54              |
| 1:B:403:VAL:HG11 | 1:B:466:THR:HB   | 1.90                     | 0.54              |
| 1:C:66:PRO:CD    | 1:C:133:ASN:HB3  | 2.37                     | 0.54              |
| 1:D:371:ILE:HB   | 1:D:380:VAL:HG13 | 1.90                     | 0.54              |
| 1:D:522:GLY:CA   | 1:D:611:THR:HG23 | 2.38                     | 0.54              |
| 1:D:564:VAL:HG11 | 1:D:667:GLN:HG2  | 1.90                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:312:THR:O    | 1:E:315:ILE:HG22 | 2.08                     | 0.54              |
| 1:F:103:PRO:HG2  | 1:F:137:ARG:HD2  | 1.89                     | 0.54              |
| 1:F:21:VAL:HG12  | 1:F:87:TYR:OH    | 2.08                     | 0.54              |
| 1:A:219:LYS:HG2  | 1:A:358:HIS:CE1  | 2.42                     | 0.54              |
| 1:A:395:PRO:HG2  | 1:A:396:PHE:CE2  | 2.44                     | 0.54              |
| 1:B:553:PRO:HB2  | 1:B:620:VAL:HG21 | 1.90                     | 0.54              |
| 1:C:215:ILE:HG12 | 1:C:353:ASP:OD2  | 2.07                     | 0.54              |
| 1:D:103:PRO:HG2  | 1:D:137:ARG:HD2  | 1.90                     | 0.54              |
| 1:F:225:HIS:HA   | 1:F:330:ALA:CB   | 2.33                     | 0.54              |
| 1:F:422:SER:HA   | 1:F:444:PHE:CZ   | 2.43                     | 0.54              |
| 1:A:197:GLU:HG2  | 1:A:201:ASP:OD2  | 2.08                     | 0.53              |
| 1:B:520:TRP:HA   | 1:B:609:SER:OG   | 2.08                     | 0.53              |
| 1:B:596:LEU:HD23 | 1:B:596:LEU:O    | 2.08                     | 0.53              |
| 1:B:729:VAL:HB   | 1:B:735:ASN:ND2  | 2.23                     | 0.53              |
| 1:C:570:LEU:HD12 | 1:C:573:VAL:CG1  | 2.38                     | 0.53              |
| 1:D:126:TYR:OH   | 1:D:185:GLY:HA3  | 2.08                     | 0.53              |
| 1:D:252:ILE:N    | 1:D:252:ILE:HD12 | 2.23                     | 0.53              |
| 1:D:488:TYR:O    | 1:D:756:LEU:HD11 | 2.08                     | 0.53              |
| 1:E:252:ILE:N    | 1:E:252:ILE:HD12 | 2.23                     | 0.53              |
| 1:F:12:VAL:HG23  | 1:F:17:PHE:CD2   | 2.44                     | 0.53              |
| 1:B:267:SER:O    | 1:B:270:GLU:HB3  | 2.07                     | 0.53              |
| 1:C:152:THR:HG21 | 1:C:360:ARG:HG3  | 1.90                     | 0.53              |
| 1:C:18:ARG:NH2   | 1:C:36:ASN:HD22  | 2.06                     | 0.53              |
| 1:C:264:ALA:CB   | 1:C:286:LYS:HA   | 2.38                     | 0.53              |
| 1:C:404:GLY:HA2  | 1:C:753:GLN:HE22 | 1.70                     | 0.53              |
| 1:C:504:ILE:HG23 | 1:C:525:LEU:O    | 2.08                     | 0.53              |
| 1:D:565:TYR:HB3  | 1:D:569:GLU:HB3  | 1.90                     | 0.53              |
| 1:E:267:SER:HB2  | 1:E:270:GLU:CB   | 2.39                     | 0.53              |
| 1:A:410:ALA:HB3  | 1:A:747:ASN:O    | 2.07                     | 0.53              |
| 1:B:286:LYS:HE3  | 1:B:290:PHE:HB2  | 1.91                     | 0.53              |
| 1:B:485:GLN:HB3  | 1:B:488:TYR:HB2  | 1.91                     | 0.53              |
| 1:B:662:VAL:O    | 1:B:665:LEU:HB3  | 2.08                     | 0.53              |
| 1:D:381:ILE:HG13 | 1:D:382:ARG:N    | 2.24                     | 0.53              |
| 1:E:205:LYS:O    | 1:E:209:LEU:HD13 | 2.08                     | 0.53              |
| 1:F:497:GLU:OE2  | 1:F:739:THR:HG22 | 2.08                     | 0.53              |
| 1:A:374:VAL:CG2  | 1:A:744:ARG:HH12 | 2.22                     | 0.53              |
| 1:B:115:GLU:HG2  | 1:B:121:ASN:ND2  | 2.24                     | 0.53              |
| 1:B:330:ALA:O    | 1:B:338:VAL:HG12 | 2.08                     | 0.53              |
| 1:B:461:HIS:CE1  | 1:B:463:ALA:HB3  | 2.43                     | 0.53              |
| 1:B:620:VAL:HG22 | 1:B:625:ALA:O    | 2.09                     | 0.53              |
| 1:C:380:VAL:HG12 | 1:C:381:ILE:H    | 1.74                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:587:TYR:CZ   | 1:F:468:LYS:HG3  | 2.43                     | 0.53              |
| 1:D:196:GLN:HG2  | 1:D:197:GLU:N    | 2.23                     | 0.53              |
| 1:D:261:LYS:HZ3  | 1:D:266:VAL:HB   | 1.73                     | 0.53              |
| 1:D:288:GLU:HB3  | 1:D:289:PRO:CD   | 2.30                     | 0.53              |
| 1:D:524:VAL:CG2  | 1:D:536:ALA:H    | 2.22                     | 0.53              |
| 1:D:653:VAL:HG11 | 1:D:689:LEU:HA   | 1.90                     | 0.53              |
| 1:E:581:ALA:HA   | 1:E:584:SER:HB3  | 1.90                     | 0.53              |
| 1:E:613:ARG:HA   | 1:E:616:ASP:OD1  | 2.09                     | 0.53              |
| 1:F:724:MSE:O    | 1:F:728:VAL:HG23 | 2.08                     | 0.53              |
| 1:F:760:TYR:HA   | 1:F:765:LEU:HB3  | 1.89                     | 0.53              |
| 1:B:292:LEU:HD11 | 1:B:324:VAL:HG21 | 1.89                     | 0.53              |
| 1:B:331:ASN:ND2  | 1:B:337:MSE:HA   | 2.18                     | 0.53              |
| 1:B:456:ILE:CG2  | 1:B:457:ILE:H    | 2.09                     | 0.53              |
| 1:D:110:ASP:O    | 1:D:113:LEU:HB3  | 2.09                     | 0.53              |
| 1:D:549:ALA:HA   | 1:D:555:ARG:HB2  | 1.89                     | 0.53              |
| 1:F:19:PRO:HG3   | 1:F:174:TYR:O    | 2.09                     | 0.53              |
| 1:F:487:HIS:O    | 1:F:491:ILE:HG12 | 2.08                     | 0.53              |
| 1:F:560:ILE:HD12 | 1:F:561:LEU:N    | 2.24                     | 0.53              |
| 1:F:580:LYS:NZ   | 1:F:590:VAL:HG22 | 2.23                     | 0.53              |
| 1:F:708:ASN:HB3  | 1:F:734:LEU:O    | 2.08                     | 0.53              |
| 1:A:267:SER:HB3  | 1:A:268:PRO:HD2  | 1.90                     | 0.53              |
| 1:B:756:LEU:O    | 1:B:759:LEU:HB3  | 2.08                     | 0.53              |
| 1:C:258:GLU:O    | 1:C:261:LYS:HG2  | 2.09                     | 0.53              |
| 1:C:468:LYS:HG3  | 1:F:587:TYR:OH   | 2.08                     | 0.53              |
| 1:D:104:PRO:HB3  | 1:D:387:PHE:O    | 2.09                     | 0.53              |
| 1:D:190:LEU:HD13 | 1:D:356:LEU:HD13 | 1.90                     | 0.53              |
| 1:D:320:SER:O    | 1:D:321:LYS:C    | 2.47                     | 0.53              |
| 1:D:247:GLN:NE2  | 1:D:637:LYS:HE3  | 2.23                     | 0.53              |
| 1:E:126:TYR:CD1  | 1:E:182:PRO:HG3  | 2.43                     | 0.53              |
| 1:E:387:PHE:O    | 1:E:390:LEU:HG   | 2.08                     | 0.53              |
| 1:E:613:ARG:HA   | 1:E:613:ARG:NE   | 2.22                     | 0.53              |
| 1:F:219:LYS:HG3  | 1:F:224:ILE:HG12 | 1.89                     | 0.53              |
| 1:F:33:TYR:OH    | 1:F:90:LYS:HE3   | 2.09                     | 0.53              |
| 1:A:15:VAL:HG12  | 1:A:16:GLY:N     | 2.21                     | 0.53              |
| 1:A:158:MSE:HE3  | 1:A:163:ARG:NH1  | 2.24                     | 0.53              |
| 1:A:330:ALA:HB1  | 1:A:348:LEU:HD21 | 1.91                     | 0.53              |
| 1:B:278:ARG:HG2  | 1:B:280:PRO:HD3  | 1.91                     | 0.53              |
| 1:C:12:VAL:HG23  | 1:C:17:PHE:CG    | 2.42                     | 0.53              |
| 1:C:380:VAL:HG12 | 1:C:381:ILE:N    | 2.24                     | 0.53              |
| 1:D:274:LEU:HB3  | 1:D:307:LEU:HD11 | 1.90                     | 0.53              |
| 1:D:329:SER:HA   | 1:D:337:MSE:HE2  | 1.89                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:339:LYS:HA   | 1:D:362:ILE:HD11 | 1.90                     | 0.53              |
| 1:A:415:LYS:C    | 1:A:417:GLY:H    | 2.11                     | 0.53              |
| 1:A:468:LYS:HG3  | 1:B:587:TYR:OH   | 2.09                     | 0.53              |
| 1:B:264:ALA:HB1  | 1:B:285:ARG:O    | 2.09                     | 0.53              |
| 1:B:487:HIS:CD2  | 1:B:520:TRP:HB3  | 2.44                     | 0.53              |
| 1:C:283:THR:HA   | 1:C:303:ILE:O    | 2.08                     | 0.53              |
| 1:C:404:GLY:HA2  | 1:C:753:GLN:CD   | 2.29                     | 0.53              |
| 1:D:380:VAL:HG12 | 1:D:381:ILE:N    | 2.24                     | 0.53              |
| 1:D:482:LEU:HD12 | 1:D:483:GLN:N    | 2.23                     | 0.53              |
| 1:D:580:LYS:HG3  | 1:D:593:ASN:ND2  | 2.23                     | 0.53              |
| 1:E:170:LEU:HD12 | 1:E:170:LEU:H    | 1.74                     | 0.53              |
| 1:E:216:VAL:HB   | 1:E:354:TYR:HB2  | 1.90                     | 0.53              |
| 1:D:601:LYS:NZ   | 1:E:771:MSE:HE3  | 2.24                     | 0.53              |
| 1:F:579:PRO:HB3  | 1:F:626:TYR:CE1  | 2.43                     | 0.53              |
| 1:A:190:LEU:HB2  | 1:A:202:PRO:HB3  | 1.90                     | 0.53              |
| 1:A:438:ARG:HG2  | 1:A:438:ARG:HH11 | 1.74                     | 0.53              |
| 1:A:543:LEU:HD12 | 1:A:549:ALA:CB   | 2.38                     | 0.53              |
| 1:A:633:GLU:H    | 1:A:634:PRO:HD2  | 1.73                     | 0.53              |
| 1:B:491:ILE:HD11 | 1:B:507:ALA:HB2  | 1.91                     | 0.53              |
| 1:C:264:ALA:HB3  | 1:C:284:LEU:HD13 | 1.91                     | 0.53              |
| 1:C:402:ALA:HB2  | 1:C:457:ILE:HB   | 1.89                     | 0.53              |
| 1:C:495:MSE:HE2  | 1:C:755:PHE:CZ   | 2.44                     | 0.53              |
| 1:D:494:VAL:HG13 | 1:D:738:VAL:H    | 1.73                     | 0.53              |
| 1:D:485:GLN:OE1  | 1:D:514:GLY:HA2  | 2.09                     | 0.53              |
| 1:E:373:PHE:CE1  | 1:E:378:ARG:HB3  | 2.44                     | 0.53              |
| 1:E:545:GLY:HA3  | 1:E:548:LEU:HB2  | 1.89                     | 0.53              |
| 1:E:661:ARG:HG3  | 1:E:663:GLU:OE2  | 2.08                     | 0.53              |
| 1:F:489:ALA:O    | 1:F:752:GLY:HA3  | 2.09                     | 0.53              |
| 1:A:156:PHE:CZ   | 1:A:186:PRO:HB3  | 2.44                     | 0.53              |
| 1:B:534:ARG:HG2  | 1:B:535:LEU:H    | 1.72                     | 0.53              |
| 1:C:15:VAL:HG12  | 1:C:16:GLY:H     | 1.74                     | 0.53              |
| 1:C:239:LEU:HD22 | 1:C:250:PHE:HE1  | 1.74                     | 0.53              |
| 1:D:193:SER:O    | 1:D:194:ASP:CB   | 2.57                     | 0.53              |
| 1:D:554:LEU:HD12 | 1:D:583:GLU:OE1  | 2.09                     | 0.53              |
| 1:D:579:PRO:O    | 1:D:582:VAL:HG23 | 2.09                     | 0.53              |
| 1:E:526:TYR:O    | 1:E:532:VAL:HG13 | 2.08                     | 0.53              |
| 1:E:572:GLY:O    | 1:E:575:ASN:HB2  | 2.09                     | 0.53              |
| 1:F:329:SER:HB2  | 1:F:331:ASN:ND2  | 2.24                     | 0.53              |
| 1:F:39:ASP:H     | 1:F:144:LEU:HD13 | 1.74                     | 0.53              |
| 1:F:759:LEU:HD11 | 1:F:764:TYR:HB2  | 1.90                     | 0.53              |
| 1:A:312:THR:O    | 1:A:316:LEU:HB2  | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:49:ARG:HD2   | 1:A:49:ARG:H     | 1.74                     | 0.52              |
| 1:A:687:LEU:HB3  | 1:A:724:MSE:HE3  | 1.90                     | 0.52              |
| 1:B:201:ASP:N    | 1:B:202:PRO:CD   | 2.71                     | 0.52              |
| 1:C:264:ALA:HB2  | 1:C:286:LYS:HA   | 1.90                     | 0.52              |
| 1:C:593:ASN:O    | 1:C:596:LEU:HB2  | 2.09                     | 0.52              |
| 1:C:651:PHE:HB2  | 1:C:688:ALA:CB   | 2.39                     | 0.52              |
| 1:D:619:ALA:HB2  | 1:D:638:LEU:HB2  | 1.91                     | 0.52              |
| 1:E:191:TYR:HB2  | 1:E:355:PHE:CB   | 2.31                     | 0.52              |
| 1:E:200:GLY:C    | 1:E:202:PRO:HD2  | 2.28                     | 0.52              |
| 1:E:522:GLY:HA3  | 1:E:538:ILE:HD12 | 1.90                     | 0.52              |
| 1:A:270:GLU:N    | 1:A:378:ARG:NH1  | 2.57                     | 0.52              |
| 1:B:522:GLY:H    | 1:B:523:GLU:CD   | 2.12                     | 0.52              |
| 1:C:379:ALA:HB3  | 1:C:744:ARG:CZ   | 2.39                     | 0.52              |
| 1:C:428:THR:HG21 | 1:C:466:THR:HG22 | 1.92                     | 0.52              |
| 1:C:461:HIS:HE1  | 1:C:463:ALA:HB3  | 1.72                     | 0.52              |
| 1:C:30:LEU:CD1   | 1:C:52:ASP:HB2   | 2.37                     | 0.52              |
| 1:D:509:ASP:CG   | 1:D:510:GLY:H    | 2.12                     | 0.52              |
| 1:D:603:ILE:HG23 | 1:E:516:ASP:HA   | 1.91                     | 0.52              |
| 1:E:617:ALA:O    | 1:E:621:LEU:HB2  | 2.09                     | 0.52              |
| 1:F:205:LYS:O    | 1:F:209:LEU:HD13 | 2.08                     | 0.52              |
| 1:F:544:PRO:HG2  | 1:F:555:ARG:HE   | 1.75                     | 0.52              |
| 1:F:57:ILE:HG13  | 1:F:75:LYS:HZ1   | 1.73                     | 0.52              |
| 1:F:738:VAL:HB   | 1:F:744:ARG:HG2  | 1.91                     | 0.52              |
| 1:A:267:SER:O    | 1:A:270:GLU:HB3  | 2.10                     | 0.52              |
| 1:A:266:VAL:HA   | 1:A:270:GLU:OE2  | 2.09                     | 0.52              |
| 1:A:695:HIS:O    | 1:A:698:VAL:HB   | 2.09                     | 0.52              |
| 1:B:565:TYR:HB3  | 1:B:569:GLU:HB3  | 1.92                     | 0.52              |
| 1:C:402:ALA:CB   | 1:C:457:ILE:HB   | 2.39                     | 0.52              |
| 1:D:183:VAL:HG23 | 1:D:184:CYS:N    | 2.24                     | 0.52              |
| 1:D:199:TYR:CG   | 1:D:200:GLY:N    | 2.77                     | 0.52              |
| 1:F:148:ARG:CZ   | 1:F:158:MSE:HG3  | 2.39                     | 0.52              |
| 1:F:192:THR:C    | 1:F:194:ASP:N    | 2.60                     | 0.52              |
| 1:F:447:ILE:O    | 1:F:447:ILE:HG22 | 2.08                     | 0.52              |
| 1:F:503:VAL:HA   | 1:F:706:VAL:HG11 | 1.91                     | 0.52              |
| 1:A:414:ALA:HA   | 1:A:418:LYS:O    | 2.10                     | 0.52              |
| 1:B:381:ILE:HG13 | 1:B:382:ARG:N    | 2.23                     | 0.52              |
| 1:B:524:VAL:CG2  | 1:B:536:ALA:H    | 2.23                     | 0.52              |
| 1:D:201:ASP:N    | 1:D:202:PRO:CD   | 2.72                     | 0.52              |
| 1:D:504:ILE:CG2  | 1:D:505:GLY:N    | 2.72                     | 0.52              |
| 1:E:391:PRO:HB3  | 1:E:420:TYR:CE1  | 2.45                     | 0.52              |
| 1:F:459:ASP:OD2  | 1:F:486:HIS:HB2  | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:641:PHE:CZ   | 1:F:678:PRO:HB2  | 2.44                     | 0.52              |
| 1:B:453:LEU:O    | 1:B:453:LEU:HG   | 2.09                     | 0.52              |
| 1:B:470:ALA:HB1  | 1:B:481:LEU:HD11 | 1.91                     | 0.52              |
| 1:B:504:ILE:CG2  | 1:B:505:GLY:N    | 2.72                     | 0.52              |
| 1:B:656:GLU:HG3  | 1:B:661:ARG:NH1  | 2.25                     | 0.52              |
| 1:C:286:LYS:NZ   | 1:C:291:PRO:HD2  | 2.25                     | 0.52              |
| 1:D:21:VAL:HA    | 1:D:24:ILE:HG22  | 1.91                     | 0.52              |
| 1:D:218:ILE:O    | 1:D:224:ILE:HB   | 2.09                     | 0.52              |
| 1:D:487:HIS:CD2  | 1:D:520:TRP:HB3  | 2.43                     | 0.52              |
| 1:D:621:LEU:HD22 | 1:D:666:PHE:HD1  | 1.75                     | 0.52              |
| 1:D:404:GLY:HA2  | 1:D:753:GLN:NE2  | 2.24                     | 0.52              |
| 1:E:102:ILE:HG12 | 1:E:144:LEU:HD11 | 1.90                     | 0.52              |
| 1:E:16:GLY:HA2   | 1:E:132:THR:OG1  | 2.08                     | 0.52              |
| 1:E:202:PRO:O    | 1:E:203:LEU:C    | 2.46                     | 0.52              |
| 1:E:37:LEU:O     | 1:E:37:LEU:HD13  | 2.10                     | 0.52              |
| 1:F:401:LEU:O    | 1:F:456:ILE:HA   | 2.08                     | 0.52              |
| 1:A:374:VAL:CG1  | 1:A:744:ARG:HH12 | 2.23                     | 0.52              |
| 1:B:371:ILE:HG13 | 1:B:380:VAL:HA   | 1.90                     | 0.52              |
| 1:B:385:ARG:HG3  | 1:B:386:GLY:H    | 1.75                     | 0.52              |
| 1:D:274:LEU:HB3  | 1:D:307:LEU:CD1  | 2.40                     | 0.52              |
| 1:D:541:TYR:CG   | 1:D:560:ILE:HG22 | 2.44                     | 0.52              |
| 1:D:543:LEU:HD12 | 1:D:549:ALA:CB   | 2.39                     | 0.52              |
| 1:E:412:GLY:HA3  | 1:E:750:ASN:ND2  | 2.21                     | 0.52              |
| 1:E:560:ILE:HD12 | 1:E:561:LEU:N    | 2.24                     | 0.52              |
| 1:F:176:ALA:O    | 1:F:179:THR:HG22 | 2.10                     | 0.52              |
| 1:F:219:LYS:HE3  | 1:F:358:HIS:CE1  | 2.45                     | 0.52              |
| 1:B:628:ARG:NH2  | 1:B:632:GLY:H    | 2.07                     | 0.52              |
| 1:C:166:TYR:CE1  | 1:C:175:HIS:HA   | 2.44                     | 0.52              |
| 1:C:579:PRO:HB3  | 1:C:626:TYR:CE1  | 2.44                     | 0.52              |
| 1:D:385:ARG:HG3  | 1:D:386:GLY:H    | 1.75                     | 0.52              |
| 1:D:78:ILE:O     | 1:D:80:PRO:HD3   | 2.09                     | 0.52              |
| 1:E:110:ASP:O    | 1:E:113:LEU:HB3  | 2.09                     | 0.52              |
| 1:E:364:ASN:HD21 | 1:E:443:HIS:CD2  | 2.27                     | 0.52              |
| 1:F:300:LEU:HA   | 1:F:640:SER:OG   | 2.10                     | 0.52              |
| 1:F:485:GLN:NE2  | 1:F:487:HIS:H    | 1.86                     | 0.52              |
| 1:A:105:ASP:CG   | 1:A:139:THR:HG23 | 2.30                     | 0.52              |
| 1:A:123:ARG:NE   | 1:A:173:ARG:NH2  | 2.58                     | 0.52              |
| 1:A:383:ARG:H    | 1:A:747:ASN:ND2  | 2.08                     | 0.52              |
| 1:A:690:ALA:HB2  | 1:A:721:ILE:HG23 | 1.91                     | 0.52              |
| 1:B:412:GLY:HA3  | 1:B:750:ASN:ND2  | 2.18                     | 0.52              |
| 1:B:594:VAL:HG12 | 1:B:594:VAL:O    | 2.10                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:207:ALA:HB1  | 1:C:320:SER:CB   | 2.34                     | 0.52              |
| 1:C:269:GLU:HB2  | 1:C:378:ARG:NH1  | 2.24                     | 0.52              |
| 1:C:409:ASN:HD22 | 1:C:425:ILE:CD1  | 2.20                     | 0.52              |
| 1:E:279:ARG:HD3  | 1:E:307:LEU:HB2  | 1.91                     | 0.52              |
| 1:F:369:SER:HB2  | 1:F:385:ARG:HB3  | 1.91                     | 0.52              |
| 1:F:429:GLY:HA2  | 1:F:465:ASN:HD22 | 1.75                     | 0.52              |
| 1:F:402:ALA:HB2  | 1:F:457:ILE:HD12 | 1.92                     | 0.52              |
| 1:F:541:TYR:CE1  | 1:F:609:SER:HA   | 2.45                     | 0.52              |
| 1:A:169:PRO:HA   | 1:A:174:TYR:CD2  | 2.45                     | 0.52              |
| 1:A:447:ILE:HG22 | 1:A:447:ILE:O    | 2.10                     | 0.52              |
| 1:B:32:GLY:H     | 1:B:87:TYR:HD2   | 1.57                     | 0.52              |
| 1:C:215:ILE:O    | 1:C:353:ASP:HB2  | 2.10                     | 0.52              |
| 1:C:666:PHE:HA   | 1:C:669:ILE:HD12 | 1.92                     | 0.52              |
| 1:C:489:ALA:HA   | 1:C:756:LEU:HD12 | 1.91                     | 0.52              |
| 1:D:451:LYS:HD3  | 1:D:477:LEU:HG   | 1.92                     | 0.52              |
| 1:E:249:PRO:HG3  | 1:E:300:LEU:CD1  | 2.37                     | 0.52              |
| 1:F:694:ALA:C    | 1:F:696:THR:H    | 2.13                     | 0.52              |
| 1:A:199:TYR:CD1  | 1:A:200:GLY:N    | 2.76                     | 0.52              |
| 1:A:254:ALA:HB1  | 1:A:259:THR:HB   | 1.92                     | 0.52              |
| 1:A:376:GLY:C    | 1:A:377:LYS:HG2  | 2.30                     | 0.52              |
| 1:A:738:VAL:HG12 | 1:A:742:VAL:O    | 2.10                     | 0.52              |
| 1:B:729:VAL:HG12 | 1:B:729:VAL:O    | 2.10                     | 0.52              |
| 1:C:288:GLU:HB2  | 1:C:289:PRO:CD   | 2.32                     | 0.52              |
| 1:C:32:GLY:O     | 1:C:87:TYR:HA    | 2.09                     | 0.52              |
| 1:D:226:LEU:HD21 | 1:D:351:VAL:HG12 | 1.91                     | 0.52              |
| 1:D:403:VAL:HG11 | 1:D:466:THR:HB   | 1.92                     | 0.52              |
| 1:D:691:ARG:HG2  | 1:D:695:HIS:CD2  | 2.45                     | 0.52              |
| 1:E:183:VAL:CG2  | 1:E:184:CYS:N    | 2.73                     | 0.52              |
| 1:E:247:GLN:HG3  | 1:E:298:PRO:CG   | 2.40                     | 0.52              |
| 1:E:269:GLU:HB2  | 1:E:378:ARG:CZ   | 2.40                     | 0.52              |
| 1:F:332:TYR:HB3  | 1:F:333:PRO:HD2  | 1.91                     | 0.52              |
| 1:A:284:LEU:HD12 | 1:A:284:LEU:O    | 2.10                     | 0.51              |
| 1:A:348:LEU:N    | 1:A:348:LEU:HD12 | 2.24                     | 0.51              |
| 1:A:714:GLY:O    | 1:A:716:ALA:N    | 2.43                     | 0.51              |
| 1:B:229:ASP:OD1  | 1:B:322:THR:HG21 | 2.10                     | 0.51              |
| 1:B:403:VAL:CG1  | 1:B:466:THR:HB   | 2.40                     | 0.51              |
| 1:B:42:VAL:O     | 1:B:42:VAL:HG13  | 2.10                     | 0.51              |
| 1:B:438:ARG:HG2  | 1:B:438:ARG:HH11 | 1.75                     | 0.51              |
| 1:B:677:SER:O    | 1:B:681:ILE:HG12 | 2.09                     | 0.51              |
| 1:C:105:ASP:OD1  | 1:C:139:THR:HG23 | 2.10                     | 0.51              |
| 1:C:370:VAL:CG2  | 1:C:381:ILE:HD11 | 2.41                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:521:GLY:CA   | 1:C:610:SER:HA   | 2.39                     | 0.51              |
| 1:C:751:VAL:HG13 | 1:C:752:GLY:N    | 2.25                     | 0.51              |
| 1:C:396:PHE:CE2  | 1:C:759:LEU:HB2  | 2.44                     | 0.51              |
| 1:D:18:ARG:HB2   | 1:D:19:PRO:HD3   | 1.91                     | 0.51              |
| 1:E:105:ASP:OD2  | 1:E:138:PHE:HB3  | 2.10                     | 0.51              |
| 1:E:306:MSE:HE1  | 1:E:368:ASP:OD2  | 2.10                     | 0.51              |
| 1:E:375:ASP:OD2  | 1:E:723:LYS:HA   | 2.10                     | 0.51              |
| 1:A:383:ARG:NH2  | 1:A:392:ILE:HD11 | 2.24                     | 0.51              |
| 1:B:15:VAL:CG1   | 1:B:67:LEU:HB2   | 2.41                     | 0.51              |
| 1:B:252:ILE:CG2  | 1:B:324:VAL:HB   | 2.41                     | 0.51              |
| 1:B:505:GLY:HA2  | 1:B:710:ALA:H    | 1.76                     | 0.51              |
| 1:C:111:ASP:CB   | 1:C:172:ARG:HH22 | 2.23                     | 0.51              |
| 1:C:408:MSE:HG3  | 1:C:424:TYR:HE1  | 1.75                     | 0.51              |
| 1:C:584:SER:CB   | 1:C:589:LYS:HB3  | 2.39                     | 0.51              |
| 1:D:558:MSE:HE2  | 1:D:574:ILE:HG13 | 1.93                     | 0.51              |
| 1:E:247:GLN:OE1  | 1:E:637:LYS:HE3  | 2.10                     | 0.51              |
| 1:F:127:PRO:HB2  | 1:F:188:TYR:HE2  | 1.75                     | 0.51              |
| 1:F:399:ASN:O    | 1:F:452:ASN:HB2  | 2.10                     | 0.51              |
| 1:A:258:GLU:O    | 1:A:261:LYS:HB2  | 2.11                     | 0.51              |
| 1:B:560:ILE:HD12 | 1:B:561:LEU:N    | 2.26                     | 0.51              |
| 1:B:620:VAL:C    | 1:B:622:LEU:N    | 2.63                     | 0.51              |
| 1:C:625:ALA:HB2  | 1:C:637:LYS:HD3  | 1.92                     | 0.51              |
| 1:D:169:PRO:HA   | 1:D:174:TYR:CD2  | 2.45                     | 0.51              |
| 1:D:603:ILE:HG22 | 1:D:604:ASN:N    | 2.25                     | 0.51              |
| 1:D:381:ILE:HG22 | 1:D:717:TYR:CZ   | 2.45                     | 0.51              |
| 1:E:168:ASP:OD1  | 1:E:169:PRO:HD2  | 2.10                     | 0.51              |
| 1:E:293:PRO:C    | 1:E:295:ASN:H    | 2.14                     | 0.51              |
| 1:E:497:GLU:OE2  | 1:E:741:GLU:HB3  | 2.10                     | 0.51              |
| 1:E:598:GLN:HG3  | 1:E:604:ASN:HD22 | 1.75                     | 0.51              |
| 1:E:766:THR:OG1  | 1:E:769:ASP:HB2  | 2.10                     | 0.51              |
| 1:E:31:ARG:HG2   | 1:E:85:ARG:O     | 2.10                     | 0.51              |
| 1:E:88:ILE:HG22  | 1:E:89:GLU:N     | 2.26                     | 0.51              |
| 1:F:690:ALA:CB   | 1:F:721:ILE:HG23 | 2.39                     | 0.51              |
| 1:F:8:VAL:C      | 1:F:9:GLN:HG3    | 2.30                     | 0.51              |
| 1:A:215:ILE:HD12 | 1:A:226:LEU:HD23 | 1.91                     | 0.51              |
| 1:A:286:LYS:HE3  | 1:A:291:PRO:HD2  | 1.92                     | 0.51              |
| 1:B:296:LEU:CD1  | 1:B:296:LEU:H    | 2.23                     | 0.51              |
| 1:B:616:ASP:OD1  | 1:B:634:PRO:HG2  | 2.10                     | 0.51              |
| 1:C:497:GLU:OE2  | 1:C:741:GLU:HB3  | 2.10                     | 0.51              |
| 1:D:209:LEU:HD23 | 1:D:354:TYR:CE2  | 2.45                     | 0.51              |
| 1:D:583:GLU:H    | 1:D:583:GLU:CD   | 2.13                     | 0.51              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:653:VAL:HG13 | 1:D:692:ALA:CB   | 2.39                     | 0.51              |
| 1:E:199:TYR:CD1  | 1:E:200:GLY:N    | 2.79                     | 0.51              |
| 1:E:593:ASN:O    | 1:E:596:LEU:HB2  | 2.11                     | 0.51              |
| 1:F:221:ILE:HG22 | 1:F:360:ARG:NH2  | 2.26                     | 0.51              |
| 1:F:488:TYR:CE1  | 1:F:525:LEU:HD13 | 2.46                     | 0.51              |
| 1:F:523:GLU:OE2  | 1:F:537:HIS:HB2  | 2.09                     | 0.51              |
| 1:F:613:ARG:HH22 | 1:F:628:ARG:NH2  | 2.09                     | 0.51              |
| 1:F:707:LYS:O    | 1:F:733:GLY:HA3  | 2.11                     | 0.51              |
| 1:A:519:THR:HB   | 1:A:608:ALA:HA   | 1.93                     | 0.51              |
| 1:B:534:ARG:C    | 1:B:535:LEU:HD12 | 2.31                     | 0.51              |
| 1:C:181:CYS:SG   | 1:C:182:PRO:N    | 2.82                     | 0.51              |
| 1:C:383:ARG:HH11 | 1:C:383:ARG:HG3  | 1.76                     | 0.51              |
| 1:D:253:MSE:HG2  | 1:D:317:PHE:HE1  | 1.75                     | 0.51              |
| 1:D:434:LEU:HD11 | 1:D:465:ASN:O    | 2.10                     | 0.51              |
| 1:D:697:ALA:HB1  | 1:D:709:VAL:HG11 | 1.93                     | 0.51              |
| 1:E:218:ILE:O    | 1:E:224:ILE:HB   | 2.11                     | 0.51              |
| 1:E:371:ILE:CD1  | 1:E:380:VAL:HG22 | 2.40                     | 0.51              |
| 1:E:503:VAL:HB   | 1:E:708:ASN:O    | 2.09                     | 0.51              |
| 1:F:124:TYR:CE2  | 1:F:125:MSE:HG2  | 2.45                     | 0.51              |
| 1:F:138:PHE:HB2  | 1:F:389:PRO:HD3  | 1.92                     | 0.51              |
| 1:F:225:HIS:HB2  | 1:F:328:THR:O    | 2.10                     | 0.51              |
| 1:F:253:MSE:HG2  | 1:F:317:PHE:CE1  | 2.45                     | 0.51              |
| 1:F:374:VAL:HG21 | 1:F:744:ARG:NH2  | 2.26                     | 0.51              |
| 1:F:495:MSE:SE   | 1:F:527:LEU:HD13 | 2.60                     | 0.51              |
| 1:A:66:PRO:HG2   | 1:A:67:LEU:H     | 1.76                     | 0.51              |
| 1:A:649:LEU:HB3  | 1:A:684:SER:HB3  | 1.92                     | 0.51              |
| 1:B:404:GLY:HA2  | 1:B:753:GLN:NE2  | 2.26                     | 0.51              |
| 1:C:487:HIS:CE1  | 1:C:512:GLY:HA3  | 2.45                     | 0.51              |
| 1:C:739:THR:HG23 | 1:C:741:GLU:H    | 1.76                     | 0.51              |
| 1:D:137:ARG:O    | 1:D:141:ILE:HG13 | 2.10                     | 0.51              |
| 1:D:3:ALA:C      | 1:D:53:ILE:HD11  | 2.31                     | 0.51              |
| 1:E:225:HIS:NE2  | 1:E:327:MSE:HE3  | 2.25                     | 0.51              |
| 1:E:538:ILE:HG23 | 1:E:662:VAL:CG2  | 2.40                     | 0.51              |
| 1:E:543:LEU:HD23 | 1:E:543:LEU:N    | 2.18                     | 0.51              |
| 1:E:663:GLU:CD   | 1:E:663:GLU:H    | 2.13                     | 0.51              |
| 1:E:12:VAL:HA    | 1:E:68:ALA:CB    | 2.40                     | 0.51              |
| 1:E:690:ALA:CB   | 1:E:721:ILE:HG23 | 2.41                     | 0.51              |
| 1:F:106:ILE:HB   | 1:F:134:CYS:HA   | 1.93                     | 0.51              |
| 1:F:267:SER:HB2  | 1:F:270:GLU:CB   | 2.39                     | 0.51              |
| 1:F:428:THR:HA   | 1:F:433:VAL:CG1  | 2.41                     | 0.51              |
| 1:F:485:GLN:OE1  | 1:F:514:GLY:HA2  | 2.10                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:491:ILE:CD1  | 1:F:525:LEU:HD12 | 2.41                     | 0.51              |
| 1:F:551:TYR:HA   | 1:F:628:ARG:HD2  | 1.91                     | 0.51              |
| 1:A:199:TYR:CG   | 1:A:200:GLY:N    | 2.79                     | 0.51              |
| 1:A:408:MSE:O    | 1:A:747:ASN:HA   | 2.11                     | 0.51              |
| 1:B:225:HIS:CA   | 1:B:330:ALA:HB2  | 2.28                     | 0.51              |
| 1:B:409:ASN:CG   | 1:B:425:ILE:HD11 | 2.30                     | 0.51              |
| 1:B:526:TYR:HB3  | 1:B:535:LEU:HD11 | 1.93                     | 0.51              |
| 1:C:144:LEU:HD23 | 1:C:145:PRO:HA   | 1.91                     | 0.51              |
| 1:C:729:VAL:HG11 | 1:C:735:ASN:HB3  | 1.91                     | 0.51              |
| 1:C:738:VAL:HB   | 1:C:744:ARG:HG2  | 1.91                     | 0.51              |
| 1:D:210:ILE:HD11 | 1:D:227:ALA:C    | 2.31                     | 0.51              |
| 1:D:424:TYR:C    | 1:D:426:GLY:H    | 2.13                     | 0.51              |
| 1:D:598:GLN:HG3  | 1:D:604:ASN:HB2  | 1.93                     | 0.51              |
| 1:D:655:VAL:HG11 | 1:D:696:THR:OG1  | 2.11                     | 0.51              |
| 1:E:153:MSE:SE   | 1:E:360:ARG:HD2  | 2.60                     | 0.51              |
| 1:E:9:GLN:NE2    | 1:E:40:ALA:HB1   | 2.25                     | 0.51              |
| 1:F:370:VAL:O    | 1:F:381:ILE:HG13 | 2.10                     | 0.51              |
| 1:F:708:ASN:HD22 | 1:F:708:ASN:N    | 2.09                     | 0.51              |
| 1:A:554:LEU:HG   | 1:A:558:MSE:HE3  | 1.93                     | 0.51              |
| 1:A:11:ILE:CG1   | 1:A:68:ALA:HA    | 2.32                     | 0.51              |
| 1:B:127:PRO:O    | 1:B:311:GLY:HA3  | 2.11                     | 0.51              |
| 1:B:409:ASN:CB   | 1:B:425:ILE:HD11 | 2.41                     | 0.51              |
| 1:B:476:GLU:O    | 1:B:477:LEU:HB3  | 2.11                     | 0.51              |
| 1:B:544:PRO:HG2  | 1:B:555:ARG:HE   | 1.75                     | 0.51              |
| 1:B:614:VAL:HG13 | 1:B:666:PHE:CE2  | 2.46                     | 0.51              |
| 1:C:590:VAL:O    | 1:C:594:VAL:HG23 | 2.10                     | 0.51              |
| 1:C:596:LEU:HD23 | 1:C:596:LEU:O    | 2.11                     | 0.51              |
| 1:D:204:ARG:HG2  | 1:D:319:TRP:CE2  | 2.46                     | 0.51              |
| 1:D:649:LEU:HB3  | 1:D:684:SER:HB3  | 1.92                     | 0.51              |
| 1:D:57:ILE:HG21  | 1:D:75:LYS:HZ1   | 1.76                     | 0.51              |
| 1:E:213:GLY:C    | 1:E:235:VAL:HG11 | 2.31                     | 0.51              |
| 1:E:392:ILE:HB   | 1:E:419:VAL:HG12 | 1.93                     | 0.51              |
| 1:E:584:SER:CB   | 1:E:589:LYS:HB3  | 2.40                     | 0.51              |
| 1:E:633:GLU:H    | 1:E:634:PRO:CD   | 2.22                     | 0.51              |
| 1:F:543:LEU:HD12 | 1:F:549:ALA:CB   | 2.40                     | 0.51              |
| 1:F:554:LEU:HG   | 1:F:620:VAL:HG11 | 1.92                     | 0.51              |
| 1:A:196:GLN:HG2  | 1:A:197:GLU:N    | 2.26                     | 0.51              |
| 1:A:406:GLU:O    | 1:A:428:THR:HG23 | 2.10                     | 0.51              |
| 1:A:424:TYR:C    | 1:A:426:GLY:H    | 2.14                     | 0.51              |
| 1:A:580:LYS:HG3  | 1:A:593:ASN:ND2  | 2.26                     | 0.51              |
| 1:C:286:LYS:HE3  | 1:C:290:PHE:HB3  | 1.93                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:31:ARG:HG2   | 1:C:85:ARG:O     | 2.10                     | 0.51              |
| 1:C:561:LEU:HB2  | 1:C:570:LEU:CD1  | 2.40                     | 0.51              |
| 1:C:633:GLU:N    | 1:C:634:PRO:HD2  | 2.26                     | 0.51              |
| 1:D:281:ILE:HG12 | 1:D:306:MSE:HG2  | 1.91                     | 0.51              |
| 1:D:33:TYR:HB2   | 1:D:88:ILE:O     | 2.11                     | 0.51              |
| 1:E:274:LEU:C    | 1:E:276:SER:H    | 2.13                     | 0.51              |
| 1:F:288:GLU:HB3  | 1:F:289:PRO:CD   | 2.32                     | 0.51              |
| 1:F:491:ILE:HD11 | 1:F:525:LEU:HD12 | 1.93                     | 0.51              |
| 1:A:278:ARG:HG3  | 1:A:280:PRO:HD3  | 1.92                     | 0.51              |
| 1:A:225:HIS:CA   | 1:A:330:ALA:HB2  | 2.39                     | 0.51              |
| 1:A:476:GLU:C    | 1:A:478:ASP:H    | 2.13                     | 0.51              |
| 1:A:593:ASN:O    | 1:A:596:LEU:HB2  | 2.10                     | 0.51              |
| 1:A:410:ALA:HB2  | 1:A:747:ASN:OD1  | 2.11                     | 0.51              |
| 1:B:522:GLY:HA3  | 1:B:611:THR:HG23 | 1.93                     | 0.51              |
| 1:D:492:ALA:O    | 1:D:495:MSE:HG2  | 2.11                     | 0.51              |
| 1:D:523:GLU:HG3  | 1:D:537:HIS:CB   | 2.41                     | 0.51              |
| 1:E:190:LEU:HB2  | 1:E:202:PRO:CB   | 2.41                     | 0.51              |
| 1:E:104:PRO:HD3  | 1:E:390:LEU:HD21 | 1.92                     | 0.51              |
| 1:E:65:PRO:C     | 1:E:67:LEU:H     | 2.14                     | 0.51              |
| 1:A:455:LEU:HA   | 1:A:479:VAL:HG12 | 1.93                     | 0.50              |
| 1:A:491:ILE:HG12 | 1:A:527:LEU:CD1  | 2.40                     | 0.50              |
| 1:A:589:LYS:HG3  | 1:A:590:VAL:HG23 | 1.92                     | 0.50              |
| 1:B:624:VAL:O    | 1:B:625:ALA:CB   | 2.58                     | 0.50              |
| 1:C:138:PHE:CG   | 1:C:389:PRO:HD3  | 2.45                     | 0.50              |
| 1:C:534:ARG:HD3  | 1:C:537:HIS:CD2  | 2.46                     | 0.50              |
| 1:D:487:HIS:CE1  | 1:D:509:ASP:HB3  | 2.46                     | 0.50              |
| 1:D:510:GLY:O    | 1:D:610:SER:HB2  | 2.11                     | 0.50              |
| 1:D:612:GLY:HA2  | 1:D:615:LEU:HD12 | 1.93                     | 0.50              |
| 1:F:308:PRO:HA   | 1:F:313:HIS:HB3  | 1.93                     | 0.50              |
| 1:F:504:ILE:HG22 | 1:F:505:GLY:H    | 1.75                     | 0.50              |
| 1:A:204:ARG:HG2  | 1:A:319:TRP:CE2  | 2.46                     | 0.50              |
| 1:A:209:LEU:HA   | 1:A:212:LYS:HB2  | 1.93                     | 0.50              |
| 1:A:543:LEU:N    | 1:A:543:LEU:HD23 | 2.26                     | 0.50              |
| 1:B:264:ALA:HB2  | 1:B:286:LYS:HA   | 1.93                     | 0.50              |
| 1:B:765:LEU:HD12 | 1:B:766:THR:H    | 1.76                     | 0.50              |
| 1:C:488:TYR:CD1  | 1:C:525:LEU:HD13 | 2.46                     | 0.50              |
| 1:C:522:GLY:HA3  | 1:C:611:THR:HG23 | 1.93                     | 0.50              |
| 1:D:102:ILE:CG2  | 1:D:389:PRO:HG3  | 2.41                     | 0.50              |
| 1:D:252:ILE:HG23 | 1:D:325:TYR:O    | 2.11                     | 0.50              |
| 1:D:13:GLN:NE2   | 1:D:42:VAL:HG23  | 2.24                     | 0.50              |
| 1:D:651:PHE:HB2  | 1:D:688:ALA:CB   | 2.42                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:751:VAL:HG13 | 1:D:752:GLY:N    | 2.26                     | 0.50              |
| 1:F:219:LYS:HB2  | 1:F:357:LEU:HA   | 1.93                     | 0.50              |
| 1:F:268:PRO:HG2  | 1:F:378:ARG:HH22 | 1.76                     | 0.50              |
| 1:F:665:LEU:O    | 1:F:669:ILE:HG13 | 2.10                     | 0.50              |
| 1:A:252:ILE:HD12 | 1:A:252:ILE:N    | 2.25                     | 0.50              |
| 1:A:281:ILE:HB   | 1:A:370:VAL:CG1  | 2.36                     | 0.50              |
| 1:A:218:ILE:HD12 | 1:A:356:LEU:HD23 | 1.93                     | 0.50              |
| 1:A:376:GLY:HA2  | 1:A:726:ARG:HH11 | 1.74                     | 0.50              |
| 1:A:373:PHE:CD2  | 1:A:378:ARG:HD3  | 2.46                     | 0.50              |
| 1:B:518:ASN:HB3  | 1:B:540:TYR:HE2  | 1.76                     | 0.50              |
| 1:B:381:ILE:HA   | 1:B:717:TYR:OH   | 2.10                     | 0.50              |
| 1:B:419:VAL:HG11 | 1:B:751:VAL:HG23 | 1.92                     | 0.50              |
| 1:C:261:LYS:HZ2  | 1:C:266:VAL:HB   | 1.75                     | 0.50              |
| 1:E:385:ARG:HG3  | 1:E:386:GLY:N    | 2.26                     | 0.50              |
| 1:E:415:LYS:C    | 1:E:417:GLY:H    | 2.13                     | 0.50              |
| 1:E:504:ILE:HG22 | 1:E:505:GLY:N    | 2.25                     | 0.50              |
| 1:F:383:ARG:HG3  | 1:F:383:ARG:HH11 | 1.76                     | 0.50              |
| 1:F:566:SER:H    | 1:F:569:GLU:HB3  | 1.77                     | 0.50              |
| 1:F:686:HIS:HE1  | 1:F:718:ASN:ND2  | 2.10                     | 0.50              |
| 1:A:106:ILE:CG2  | 1:A:277:TYR:HB2  | 2.37                     | 0.50              |
| 1:A:370:VAL:CG2  | 1:A:381:ILE:HD11 | 2.41                     | 0.50              |
| 1:B:35:LYS:HG3   | 1:B:90:LYS:HB3   | 1.92                     | 0.50              |
| 1:B:537:HIS:HB3  | 1:B:659:LEU:HD23 | 1.92                     | 0.50              |
| 1:B:65:PRO:C     | 1:B:67:LEU:H     | 2.13                     | 0.50              |
| 1:C:142:GLU:HB2  | 1:C:150:ASN:C    | 2.32                     | 0.50              |
| 1:C:245:ARG:NE   | 1:C:250:PHE:HE2  | 2.09                     | 0.50              |
| 1:C:251:ALA:O    | 1:C:326:VAL:HA   | 2.11                     | 0.50              |
| 1:C:504:ILE:HD12 | 1:C:701:ALA:HB2  | 1.93                     | 0.50              |
| 1:D:65:PRO:HG2   | 1:D:68:ALA:HB3   | 1.92                     | 0.50              |
| 1:D:394:ILE:HG23 | 1:D:755:PHE:HB2  | 1.93                     | 0.50              |
| 1:D:587:TYR:OH   | 1:E:468:LYS:HG3  | 2.11                     | 0.50              |
| 1:F:406:GLU:HG3  | 1:F:407:LEU:N    | 2.27                     | 0.50              |
| 1:F:610:SER:O    | 1:F:614:VAL:HG23 | 2.12                     | 0.50              |
| 1:A:319:TRP:O    | 1:A:320:SER:HB3  | 2.11                     | 0.50              |
| 1:A:486:HIS:O    | 1:A:489:ALA:HB3  | 2.10                     | 0.50              |
| 1:A:743:PRO:HG3  | 1:A:747:ASN:HD22 | 1.76                     | 0.50              |
| 1:B:158:MSE:HE3  | 1:B:163:ARG:NH1  | 2.27                     | 0.50              |
| 1:B:1:MSE:HE2    | 1:B:47:GLU:C     | 2.32                     | 0.50              |
| 1:C:399:ASN:O    | 1:C:454:ASP:HB2  | 2.11                     | 0.50              |
| 1:D:28:HIS:CD2   | 1:D:56:PHE:HB2   | 2.47                     | 0.50              |
| 1:D:323:PRO:HG2  | 1:D:324:VAL:H    | 1.77                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:371:ILE:CG1  | 1:D:380:VAL:HG22 | 2.42                     | 0.50              |
| 1:D:508:LEU:HB3  | 1:D:715:VAL:HB   | 1.94                     | 0.50              |
| 1:D:748:GLY:O    | 1:D:751:VAL:HG12 | 2.11                     | 0.50              |
| 1:E:163:ARG:O    | 1:E:167:GLU:HG2  | 2.10                     | 0.50              |
| 1:F:189:ARG:HD2  | 1:F:191:TYR:OH   | 2.11                     | 0.50              |
| 1:F:456:ILE:O    | 1:F:482:LEU:HB3  | 2.12                     | 0.50              |
| 1:F:504:ILE:HD11 | 1:F:701:ALA:HA   | 1.93                     | 0.50              |
| 1:F:756:LEU:HD21 | 1:F:770:LEU:HD22 | 1.93                     | 0.50              |
| 1:A:111:ASP:CB   | 1:A:172:ARG:HH22 | 2.25                     | 0.50              |
| 1:A:65:PRO:HG2   | 1:A:68:ALA:CB    | 2.42                     | 0.50              |
| 1:B:399:ASN:O    | 1:B:454:ASP:HB2  | 2.11                     | 0.50              |
| 1:C:138:PHE:HA   | 1:C:141:ILE:HD12 | 1.94                     | 0.50              |
| 1:C:498:LYS:HB2  | 1:C:500:LEU:HD12 | 1.94                     | 0.50              |
| 1:C:247:GLN:HE22 | 1:C:637:LYS:NZ   | 2.09                     | 0.50              |
| 1:D:253:MSE:HE2  | 1:D:317:PHE:CE1  | 2.46                     | 0.50              |
| 1:E:192:THR:HG23 | 1:E:353:ASP:O    | 2.12                     | 0.50              |
| 1:E:219:LYS:HG3  | 1:E:224:ILE:CG2  | 2.41                     | 0.50              |
| 1:E:523:GLU:OE2  | 1:E:537:HIS:HB2  | 2.11                     | 0.50              |
| 1:E:32:GLY:O     | 1:E:87:TYR:HA    | 2.11                     | 0.50              |
| 1:F:140:ILE:HG21 | 1:F:360:ARG:NH1  | 2.26                     | 0.50              |
| 1:F:232:ASN:OD1  | 1:F:234:GLU:HB3  | 2.11                     | 0.50              |
| 1:F:582:VAL:HG21 | 1:F:626:TYR:CD1  | 2.46                     | 0.50              |
| 1:B:396:PHE:CE2  | 1:B:759:LEU:HB2  | 2.47                     | 0.50              |
| 1:C:263:PHE:HE1  | 1:C:292:LEU:HB2  | 1.76                     | 0.50              |
| 1:D:267:SER:O    | 1:D:270:GLU:HB3  | 2.11                     | 0.50              |
| 1:D:292:LEU:HB3  | 1:D:296:LEU:HD22 | 1.92                     | 0.50              |
| 1:D:504:ILE:H    | 1:D:706:VAL:HG11 | 1.77                     | 0.50              |
| 1:E:284:LEU:O    | 1:E:302:THR:HA   | 2.11                     | 0.50              |
| 1:E:535:LEU:HD23 | 1:E:700:ARG:HG3  | 1.93                     | 0.50              |
| 1:E:714:GLY:C    | 1:E:716:ALA:H    | 2.14                     | 0.50              |
| 1:F:4:TYR:HA     | 1:F:76:LYS:O     | 2.11                     | 0.50              |
| 1:C:181:CYS:SG   | 1:C:183:VAL:HG13 | 2.51                     | 0.50              |
| 1:A:724:MSE:HE1  | 1:C:289:PRO:HB3  | 1.94                     | 0.50              |
| 1:D:219:LYS:HA   | 1:D:224:ILE:HG22 | 1.94                     | 0.50              |
| 1:D:279:ARG:HD3  | 1:D:307:LEU:HB2  | 1.93                     | 0.50              |
| 1:D:300:LEU:CD2  | 1:D:636:MSE:HE2  | 2.42                     | 0.50              |
| 1:D:456:ILE:HD11 | 1:D:479:VAL:HB   | 1.94                     | 0.50              |
| 1:D:497:GLU:OE1  | 1:D:738:VAL:HA   | 2.11                     | 0.50              |
| 1:D:641:PHE:HZ   | 1:D:678:PRO:HB2  | 1.76                     | 0.50              |
| 1:E:213:GLY:CA   | 1:E:235:VAL:HG11 | 2.42                     | 0.50              |
| 1:E:36:ASN:HA    | 1:E:41:GLY:O     | 2.12                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:456:ILE:HG22 | 1:E:457:ILE:H    | 1.77                     | 0.50              |
| 1:E:485:GLN:CG   | 1:E:488:TYR:H    | 2.23                     | 0.50              |
| 1:E:582:VAL:CG1  | 1:E:626:TYR:HB3  | 2.40                     | 0.50              |
| 1:F:140:ILE:HB   | 1:F:152:THR:CG2  | 2.42                     | 0.50              |
| 1:F:233:GLU:HB2  | 1:F:293:PRO:HB3  | 1.93                     | 0.50              |
| 1:F:476:GLU:C    | 1:F:478:ASP:H    | 2.14                     | 0.50              |
| 1:A:177:GLU:HB2  | 1:A:178:PRO:HD3  | 1.93                     | 0.50              |
| 1:A:582:VAL:C    | 1:A:584:SER:H    | 2.14                     | 0.50              |
| 1:A:765:LEU:CD2  | 1:A:770:LEU:HD21 | 2.41                     | 0.50              |
| 1:B:315:ILE:HG23 | 1:B:316:LEU:N    | 2.26                     | 0.50              |
| 1:B:528:GLY:N    | 1:B:532:VAL:HG22 | 2.27                     | 0.50              |
| 1:C:477:LEU:HB3  | 1:C:479:VAL:HG23 | 1.94                     | 0.50              |
| 1:C:15:VAL:HG11  | 1:C:67:LEU:HB2   | 1.94                     | 0.50              |
| 1:C:709:VAL:O    | 1:C:735:ASN:HB2  | 2.12                     | 0.50              |
| 1:D:383:ARG:HD2  | 1:D:387:PHE:CD2  | 2.46                     | 0.50              |
| 1:D:613:ARG:HA   | 1:D:613:ARG:NE   | 2.27                     | 0.50              |
| 1:E:16:GLY:C     | 1:E:19:PRO:HD2   | 2.32                     | 0.50              |
| 1:E:236:VAL:HG21 | 1:E:296:LEU:HD12 | 1.94                     | 0.50              |
| 1:E:396:PHE:CZ   | 1:E:759:LEU:HD13 | 2.46                     | 0.50              |
| 1:F:253:MSE:HG2  | 1:F:317:PHE:HE1  | 1.76                     | 0.50              |
| 1:F:35:LYS:HE2   | 1:F:90:LYS:HZ2   | 1.76                     | 0.50              |
| 1:F:380:VAL:HG21 | 1:F:740:THR:HG23 | 1.94                     | 0.50              |
| 1:A:189:ARG:HA   | 1:A:202:PRO:HG3  | 1.94                     | 0.49              |
| 1:A:427:ASN:O    | 1:A:433:VAL:HG21 | 2.11                     | 0.49              |
| 1:A:456:ILE:CG2  | 1:A:457:ILE:N    | 2.72                     | 0.49              |
| 1:A:557:LEU:HD23 | 1:A:557:LEU:O    | 2.12                     | 0.49              |
| 1:A:381:ILE:HG22 | 1:A:717:TYR:CZ   | 2.47                     | 0.49              |
| 1:B:543:LEU:H    | 1:B:543:LEU:HD23 | 1.77                     | 0.49              |
| 1:C:123:ARG:HH22 | 1:C:173:ARG:HG2  | 1.76                     | 0.49              |
| 1:C:224:ILE:HG22 | 1:C:338:VAL:O    | 2.12                     | 0.49              |
| 1:C:315:ILE:CG2  | 1:C:316:LEU:N    | 2.75                     | 0.49              |
| 1:C:427:ASN:O    | 1:C:433:VAL:HG11 | 2.12                     | 0.49              |
| 1:D:281:ILE:HG12 | 1:D:306:MSE:CG   | 2.42                     | 0.49              |
| 1:E:233:GLU:O    | 1:E:236:VAL:HG12 | 2.12                     | 0.49              |
| 1:E:188:TYR:OH   | 1:E:312:THR:HG21 | 2.12                     | 0.49              |
| 1:E:230:ALA:HB3  | 1:E:324:VAL:HG23 | 1.94                     | 0.49              |
| 1:E:457:ILE:HG22 | 1:E:458:ALA:N    | 2.27                     | 0.49              |
| 1:D:589:LYS:H    | 1:E:475:ASN:ND2  | 2.10                     | 0.49              |
| 1:E:722:THR:O    | 1:E:726:ARG:HB2  | 2.11                     | 0.49              |
| 1:A:230:ALA:HB2  | 1:A:326:VAL:CG2  | 2.36                     | 0.49              |
| 1:A:286:LYS:HE3  | 1:A:291:PRO:CD   | 2.43                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:399:ASN:ND2  | 1:A:399:ASN:N    | 2.60                     | 0.49              |
| 1:A:61:TYR:CE2   | 1:A:73:ILE:HD12  | 2.46                     | 0.49              |
| 1:B:515:THR:O    | 1:B:516:ASP:HB2  | 2.12                     | 0.49              |
| 1:C:266:VAL:HG22 | 1:C:284:LEU:HD22 | 1.93                     | 0.49              |
| 1:C:306:MSE:HE1  | 1:C:368:ASP:OD2  | 2.12                     | 0.49              |
| 1:C:415:LYS:C    | 1:C:417:GLY:H    | 2.15                     | 0.49              |
| 1:C:633:GLU:H    | 1:C:634:PRO:HD2  | 1.77                     | 0.49              |
| 1:D:329:SER:HB3  | 1:D:337:MSE:HE2  | 1.94                     | 0.49              |
| 1:D:475:ASN:ND2  | 1:E:589:LYS:H    | 2.09                     | 0.49              |
| 1:A:409:ASN:ND2  | 1:A:425:ILE:HD11 | 2.27                     | 0.49              |
| 1:A:639:GLU:OE2  | 1:A:718:ASN:HA   | 2.13                     | 0.49              |
| 1:B:22:TYR:CE1   | 1:B:87:TYR:HB3   | 2.47                     | 0.49              |
| 1:B:379:ALA:HB2  | 1:B:737:HIS:HE1  | 1.77                     | 0.49              |
| 1:B:409:ASN:HB3  | 1:B:425:ILE:HD11 | 1.93                     | 0.49              |
| 1:C:130:VAL:HG23 | 1:C:134:CYS:SG   | 2.53                     | 0.49              |
| 1:C:220:GLY:H    | 1:C:224:ILE:HA   | 1.78                     | 0.49              |
| 1:C:406:GLU:HA   | 1:C:466:THR:CG2  | 2.42                     | 0.49              |
| 1:C:540:TYR:HA   | 1:C:608:ALA:O    | 2.12                     | 0.49              |
| 1:C:586:LYS:CB   | 1:C:627:ARG:HH22 | 2.25                     | 0.49              |
| 1:C:20:PHE:HE1   | 1:C:60:LEU:HD12  | 1.77                     | 0.49              |
| 1:C:649:LEU:CD1  | 1:C:650:LYS:H    | 2.24                     | 0.49              |
| 1:D:394:ILE:HG22 | 1:D:396:PHE:H    | 1.76                     | 0.49              |
| 1:D:456:ILE:HD12 | 1:D:480:GLU:O    | 2.12                     | 0.49              |
| 1:E:278:ARG:HG3  | 1:E:280:PRO:HD3  | 1.94                     | 0.49              |
| 1:E:398:TYR:CZ   | 1:E:758:GLY:HA3  | 2.48                     | 0.49              |
| 1:E:759:LEU:CD1  | 1:E:764:TYR:HB2  | 2.42                     | 0.49              |
| 1:F:714:GLY:C    | 1:F:716:ALA:H    | 2.16                     | 0.49              |
| 1:A:111:ASP:HB3  | 1:A:172:ARG:NH1  | 2.25                     | 0.49              |
| 1:A:148:ARG:NH1  | 1:A:158:MSE:HG3  | 2.27                     | 0.49              |
| 1:B:398:TYR:OH   | 1:B:754:ALA:HA   | 2.13                     | 0.49              |
| 1:B:593:ASN:C    | 1:B:595:VAL:H    | 2.16                     | 0.49              |
| 1:B:633:GLU:N    | 1:B:634:PRO:HD2  | 2.23                     | 0.49              |
| 1:C:287:LYS:CG   | 1:C:289:PRO:HD2  | 2.40                     | 0.49              |
| 1:D:149:GLU:O    | 1:D:154:LYS:HG3  | 2.12                     | 0.49              |
| 1:D:286:LYS:HD2  | 1:D:303:ILE:HD11 | 1.94                     | 0.49              |
| 1:D:472:GLU:O    | 1:D:476:GLU:HG2  | 2.13                     | 0.49              |
| 1:E:458:ALA:HB1  | 1:E:467:THR:HG22 | 1.94                     | 0.49              |
| 1:F:16:GLY:C     | 1:F:19:PRO:HD2   | 2.32                     | 0.49              |
| 1:F:201:ASP:N    | 1:F:202:PRO:CD   | 2.75                     | 0.49              |
| 1:F:204:ARG:O    | 1:F:208:GLU:HG3  | 2.13                     | 0.49              |
| 1:F:338:VAL:HG23 | 1:F:343:ARG:HB2  | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:488:TYR:CE1  | 1:A:525:LEU:HD13 | 2.47                     | 0.49              |
| 1:A:504:ILE:HD12 | 1:A:701:ALA:HA   | 1.94                     | 0.49              |
| 1:C:12:VAL:HG13  | 1:C:13:GLN:CD    | 2.33                     | 0.49              |
| 1:C:320:SER:O    | 1:C:322:THR:N    | 2.44                     | 0.49              |
| 1:C:565:TYR:HB3  | 1:C:569:GLU:HB3  | 1.93                     | 0.49              |
| 1:C:760:TYR:HA   | 1:C:765:LEU:HB3  | 1.93                     | 0.49              |
| 1:D:257:ILE:CD1  | 1:D:271:GLU:HG3  | 2.43                     | 0.49              |
| 1:D:766:THR:OG1  | 1:D:769:ASP:HB2  | 2.11                     | 0.49              |
| 1:E:428:THR:HA   | 1:E:433:VAL:CG1  | 2.41                     | 0.49              |
| 1:F:280:PRO:HB2  | 1:F:371:ILE:HG22 | 1.95                     | 0.49              |
| 1:F:504:ILE:CG2  | 1:F:505:GLY:N    | 2.76                     | 0.49              |
| 1:C:601:LYS:HZ2  | 1:F:771:MSE:HE3  | 1.76                     | 0.49              |
| 1:A:210:ILE:HD11 | 1:A:228:CYS:CA   | 2.43                     | 0.49              |
| 1:A:369:SER:H    | 1:A:385:ARG:CB   | 2.26                     | 0.49              |
| 1:A:445:ARG:HH21 | 1:A:452:ASN:HD22 | 1.58                     | 0.49              |
| 1:A:490:HIS:CG   | 1:A:713:GLY:HA2  | 2.48                     | 0.49              |
| 1:B:191:TYR:CD1  | 1:B:196:GLN:HB3  | 2.48                     | 0.49              |
| 1:B:205:LYS:O    | 1:B:209:LEU:HD13 | 2.12                     | 0.49              |
| 1:B:279:ARG:CB   | 1:B:309:TYR:HB3  | 2.41                     | 0.49              |
| 1:B:549:ALA:HA   | 1:B:555:ARG:CB   | 2.42                     | 0.49              |
| 1:C:216:VAL:HG23 | 1:C:354:TYR:O    | 2.12                     | 0.49              |
| 1:D:415:LYS:HD2  | 1:D:448:LEU:HD22 | 1.95                     | 0.49              |
| 1:D:399:ASN:O    | 1:D:452:ASN:HB2  | 2.12                     | 0.49              |
| 1:D:506:ILE:HB   | 1:D:711:LEU:CD1  | 2.43                     | 0.49              |
| 1:D:15:VAL:HG21  | 1:D:67:LEU:O     | 2.13                     | 0.49              |
| 1:E:370:VAL:HG22 | 1:E:382:ARG:HD2  | 1.94                     | 0.49              |
| 1:E:541:TYR:OH   | 1:E:610:SER:O    | 2.30                     | 0.49              |
| 1:E:583:GLU:HG3  | 1:E:592:PHE:CD1  | 2.47                     | 0.49              |
| 1:E:613:ARG:HA   | 1:E:613:ARG:HE   | 1.78                     | 0.49              |
| 1:F:111:ASP:HB3  | 1:F:172:ARG:HH12 | 1.76                     | 0.49              |
| 1:F:137:ARG:O    | 1:F:141:ILE:HG13 | 2.13                     | 0.49              |
| 1:A:19:PRO:O     | 1:A:23:ARG:HG3   | 2.13                     | 0.49              |
| 1:A:217:ALA:HB1  | 1:A:224:ILE:CD1  | 2.41                     | 0.49              |
| 1:A:225:HIS:HB2  | 1:A:328:THR:O    | 2.12                     | 0.49              |
| 1:B:278:ARG:NH1  | 1:B:387:PHE:HE1  | 2.10                     | 0.49              |
| 1:B:408:MSE:HG3  | 1:B:424:TYR:HE1  | 1.76                     | 0.49              |
| 1:B:545:GLY:HA3  | 1:B:548:LEU:HB2  | 1.95                     | 0.49              |
| 1:A:475:ASN:ND2  | 1:B:589:LYS:N    | 2.60                     | 0.49              |
| 1:C:370:VAL:O    | 1:C:381:ILE:HG13 | 2.12                     | 0.49              |
| 1:C:429:GLY:HA2  | 1:C:465:ASN:HD22 | 1.77                     | 0.49              |
| 1:D:660:ILE:HG22 | 1:D:662:VAL:HG23 | 1.94                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:708:ASN:HB3  | 1:D:734:LEU:O    | 2.13                     | 0.49              |
| 1:D:375:ASP:OD2  | 1:D:723:LYS:HA   | 2.13                     | 0.49              |
| 1:D:743:PRO:HG2  | 1:D:748:GLY:HA3  | 1.95                     | 0.49              |
| 1:E:210:ILE:HD13 | 1:E:216:VAL:CG1  | 2.37                     | 0.49              |
| 1:E:282:ILE:HG23 | 1:E:283:THR:N    | 2.26                     | 0.49              |
| 1:E:227:ALA:HA   | 1:E:326:VAL:O    | 2.13                     | 0.49              |
| 1:F:334:GLY:HA3  | 1:F:335:MSE:HE2  | 1.93                     | 0.49              |
| 1:F:413:VAL:HG13 | 1:F:420:TYR:HB2  | 1.95                     | 0.49              |
| 1:A:331:ASN:ND2  | 1:A:337:MSE:HA   | 2.23                     | 0.49              |
| 1:B:495:MSE:SE   | 1:B:527:LEU:HD13 | 2.63                     | 0.49              |
| 1:B:529:TYR:HD1  | 1:B:764:TYR:HB3  | 1.78                     | 0.49              |
| 1:B:508:LEU:CD2  | 1:B:611:THR:HG21 | 2.41                     | 0.49              |
| 1:C:11:ILE:HG21  | 1:C:69:ARG:N     | 2.23                     | 0.49              |
| 1:C:170:LEU:HD12 | 1:C:170:LEU:N    | 2.27                     | 0.49              |
| 1:C:232:ASN:OD1  | 1:C:235:VAL:HG22 | 2.13                     | 0.49              |
| 1:C:485:GLN:OE1  | 1:C:514:GLY:HA2  | 2.13                     | 0.49              |
| 1:D:116:LEU:HD23 | 1:D:129:ILE:HG21 | 1.95                     | 0.49              |
| 1:E:196:GLN:NE2  | 1:E:196:GLN:N    | 2.61                     | 0.49              |
| 1:E:255:LYS:HG2  | 1:E:256:ASP:OD2  | 2.13                     | 0.49              |
| 1:E:384:SER:HA   | 1:E:388:VAL:HG23 | 1.93                     | 0.49              |
| 1:E:24:ILE:HG23  | 1:E:56:PHE:CE1   | 2.47                     | 0.49              |
| 1:E:757:GLY:C    | 1:E:759:LEU:H    | 2.16                     | 0.49              |
| 1:F:159:CYS:SG   | 1:F:183:VAL:HG21 | 2.53                     | 0.49              |
| 1:F:237:ALA:HA   | 1:F:295:ASN:HD21 | 1.77                     | 0.49              |
| 1:F:385:ARG:HG3  | 1:F:386:GLY:N    | 2.28                     | 0.49              |
| 1:F:457:ILE:HG21 | 1:F:753:GLN:HB3  | 1.95                     | 0.49              |
| 1:A:107:ALA:O    | 1:A:134:CYS:HB2  | 2.11                     | 0.49              |
| 1:A:404:GLY:HA2  | 1:A:753:GLN:CD   | 2.33                     | 0.49              |
| 1:B:193:SER:O    | 1:B:194:ASP:CB   | 2.60                     | 0.49              |
| 1:B:495:MSE:HG3  | 1:B:755:PHE:CZ   | 2.47                     | 0.49              |
| 1:C:163:ARG:HA   | 1:C:166:TYR:HB3  | 1.95                     | 0.49              |
| 1:C:28:HIS:HB3   | 1:C:52:ASP:HB3   | 1.95                     | 0.49              |
| 1:D:491:ILE:HD11 | 1:D:505:GLY:CA   | 2.41                     | 0.49              |
| 1:E:738:VAL:CG1  | 1:E:742:VAL:HB   | 2.41                     | 0.49              |
| 1:E:9:GLN:HE21   | 1:E:40:ALA:HB1   | 1.77                     | 0.49              |
| 1:F:242:ARG:HH22 | 1:F:353:ASP:CG   | 2.17                     | 0.49              |
| 1:A:464:TYR:C    | 1:A:466:THR:N    | 2.67                     | 0.49              |
| 1:A:751:VAL:HG13 | 1:A:752:GLY:N    | 2.27                     | 0.49              |
| 1:B:31:ARG:HB3   | 1:B:86:PHE:O     | 2.13                     | 0.49              |
| 1:B:495:MSE:SE   | 1:B:527:LEU:HD22 | 2.63                     | 0.49              |
| 1:C:190:LEU:HB2  | 1:C:202:PRO:CB   | 2.39                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:309:TYR:CG   | 1:C:385:ARG:NH2  | 2.81                     | 0.49              |
| 1:C:433:VAL:O    | 1:C:436:PHE:HB3  | 2.12                     | 0.49              |
| 1:D:104:PRO:O    | 1:D:137:ARG:HB2  | 2.12                     | 0.49              |
| 1:F:181:CYS:SG   | 1:F:182:PRO:N    | 2.85                     | 0.49              |
| 1:F:725:ILE:O    | 1:F:729:VAL:HG23 | 2.13                     | 0.49              |
| 1:A:545:GLY:HA3  | 1:A:548:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:557:LEU:HD12 | 1:A:620:VAL:HB   | 1.94                     | 0.48              |
| 1:A:655:VAL:HG22 | 1:A:660:ILE:HG12 | 1.94                     | 0.48              |
| 1:C:130:VAL:HG22 | 1:C:131:CYS:N    | 2.28                     | 0.48              |
| 1:C:130:VAL:HG11 | 1:C:178:PRO:O    | 2.13                     | 0.48              |
| 1:C:210:ILE:HG21 | 1:C:325:TYR:HE1  | 1.77                     | 0.48              |
| 1:C:218:ILE:C    | 1:C:224:ILE:HG13 | 2.33                     | 0.48              |
| 1:C:566:SER:N    | 1:C:569:GLU:HB2  | 2.27                     | 0.48              |
| 1:D:376:GLY:C    | 1:D:377:LYS:HD2  | 2.33                     | 0.48              |
| 1:D:509:ASP:CG   | 1:D:510:GLY:N    | 2.66                     | 0.48              |
| 1:D:515:THR:O    | 1:D:516:ASP:HB2  | 2.12                     | 0.48              |
| 1:D:519:THR:HB   | 1:D:608:ALA:CA   | 2.37                     | 0.48              |
| 1:E:113:LEU:O    | 1:E:116:LEU:HG   | 2.13                     | 0.48              |
| 1:E:370:VAL:HG23 | 1:E:381:ILE:HG13 | 1.95                     | 0.48              |
| 1:F:22:TYR:CD2   | 1:F:169:PRO:HB3  | 2.48                     | 0.48              |
| 1:F:4:TYR:CB     | 1:F:53:ILE:HD11  | 2.43                     | 0.48              |
| 1:F:7:HIS:CD2    | 1:F:43:GLU:HB3   | 2.48                     | 0.48              |
| 1:A:251:ALA:HB3  | 1:A:327:MSE:O    | 2.14                     | 0.48              |
| 1:A:502:SER:CB   | 1:A:528:GLY:HA2  | 2.43                     | 0.48              |
| 1:B:516:ASP:C    | 1:B:518:ASN:H    | 2.17                     | 0.48              |
| 1:C:24:ILE:HG23  | 1:C:56:PHE:CE1   | 2.47                     | 0.48              |
| 1:C:256:ASP:O    | 1:C:257:ILE:C    | 2.52                     | 0.48              |
| 1:D:219:LYS:HA   | 1:D:224:ILE:HB   | 1.95                     | 0.48              |
| 1:D:274:LEU:C    | 1:D:276:SER:H    | 2.17                     | 0.48              |
| 1:D:398:TYR:HB2  | 1:D:454:ASP:CG   | 2.33                     | 0.48              |
| 1:D:677:SER:O    | 1:D:681:ILE:HG12 | 2.13                     | 0.48              |
| 1:E:219:LYS:HD3  | 1:E:358:HIS:H    | 1.76                     | 0.48              |
| 1:F:146:TYR:CE1  | 1:F:177:GLU:HG2  | 2.49                     | 0.48              |
| 1:F:601:LYS:CB   | 1:F:603:ILE:HG13 | 2.43                     | 0.48              |
| 1:A:239:LEU:HD22 | 1:A:250:PHE:HZ   | 1.77                     | 0.48              |
| 1:A:450:VAL:HG22 | 1:A:451:LYS:N    | 2.28                     | 0.48              |
| 1:B:16:GLY:HA2   | 1:B:132:THR:OG1  | 2.12                     | 0.48              |
| 1:C:225:HIS:N    | 1:C:225:HIS:CD2  | 2.81                     | 0.48              |
| 1:C:270:GLU:N    | 1:C:378:ARG:NH1  | 2.62                     | 0.48              |
| 1:D:392:ILE:N    | 1:D:392:ILE:HD12 | 2.29                     | 0.48              |
| 1:E:510:GLY:O    | 1:E:511:VAL:HG23 | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:124:TYR:O    | 1:F:125:MSE:HB2  | 2.13                     | 0.48              |
| 1:F:216:VAL:O    | 1:F:227:ALA:HB3  | 2.13                     | 0.48              |
| 1:F:31:ARG:HB3   | 1:F:86:PHE:O     | 2.12                     | 0.48              |
| 1:A:116:LEU:C    | 1:A:118:ASP:H    | 2.17                     | 0.48              |
| 1:A:144:LEU:HD23 | 1:A:146:TYR:N    | 2.27                     | 0.48              |
| 1:B:216:VAL:O    | 1:B:227:ALA:HB3  | 2.13                     | 0.48              |
| 1:B:406:GLU:HA   | 1:B:466:THR:HG21 | 1.96                     | 0.48              |
| 1:B:427:ASN:O    | 1:B:433:VAL:HG11 | 2.13                     | 0.48              |
| 1:C:375:ASP:OD2  | 1:C:723:LYS:HA   | 2.13                     | 0.48              |
| 1:D:543:LEU:CD2  | 1:D:543:LEU:H    | 2.20                     | 0.48              |
| 1:D:557:LEU:HD23 | 1:D:557:LEU:O    | 2.13                     | 0.48              |
| 1:D:714:GLY:C    | 1:D:716:ALA:H    | 2.16                     | 0.48              |
| 1:E:144:LEU:CD1  | 1:E:447:ILE:HG23 | 2.40                     | 0.48              |
| 1:E:456:ILE:O    | 1:E:482:LEU:HB3  | 2.13                     | 0.48              |
| 1:F:300:LEU:HD22 | 1:F:636:MSE:HE2  | 1.95                     | 0.48              |
| 1:F:315:ILE:HG23 | 1:F:316:LEU:N    | 2.28                     | 0.48              |
| 1:F:383:ARG:CZ   | 1:F:421:PRO:HG3  | 2.43                     | 0.48              |
| 1:A:253:MSE:HA   | 1:A:306:MSE:O    | 2.13                     | 0.48              |
| 1:A:309:TYR:CZ   | 1:A:313:HIS:NE2  | 2.81                     | 0.48              |
| 1:B:170:LEU:H    | 1:B:170:LEU:HD12 | 1.79                     | 0.48              |
| 1:C:21:VAL:HA    | 1:C:24:ILE:CG2   | 2.42                     | 0.48              |
| 1:C:253:MSE:HG3  | 1:C:306:MSE:O    | 2.14                     | 0.48              |
| 1:C:317:PHE:CE2  | 1:C:323:PRO:HA   | 2.45                     | 0.48              |
| 1:C:9:GLN:NE2    | 1:C:40:ALA:HB1   | 2.28                     | 0.48              |
| 1:D:170:LEU:N    | 1:D:170:LEU:HD12 | 2.25                     | 0.48              |
| 1:D:399:ASN:HA   | 1:D:414:ALA:O    | 2.13                     | 0.48              |
| 1:E:265:TYR:O    | 1:E:284:LEU:HD22 | 2.13                     | 0.48              |
| 1:E:539:ASP:CA   | 1:E:659:LEU:HD11 | 2.40                     | 0.48              |
| 1:F:11:ILE:O     | 1:F:11:ILE:HG23  | 2.12                     | 0.48              |
| 1:F:15:VAL:C     | 1:F:17:PHE:H     | 2.17                     | 0.48              |
| 1:F:182:PRO:HB3  | 1:F:199:TYR:OH   | 2.14                     | 0.48              |
| 1:F:490:HIS:C    | 1:F:492:ALA:H    | 2.17                     | 0.48              |
| 1:A:380:VAL:CG1  | 1:A:381:ILE:H    | 2.15                     | 0.48              |
| 1:A:445:ARG:HH22 | 1:A:477:LEU:HD22 | 1.77                     | 0.48              |
| 1:A:495:MSE:HG3  | 1:A:755:PHE:CE2  | 2.48                     | 0.48              |
| 1:B:588:GLY:O    | 1:B:592:PHE:HD2  | 1.97                     | 0.48              |
| 1:B:691:ARG:HD3  | 1:B:724:MSE:HE3  | 1.93                     | 0.48              |
| 1:B:725:ILE:O    | 1:B:729:VAL:HG23 | 2.13                     | 0.48              |
| 1:C:105:ASP:HA   | 1:C:137:ARG:HB2  | 1.94                     | 0.48              |
| 1:C:265:TYR:CE2  | 1:C:287:LYS:HD2  | 2.47                     | 0.48              |
| 1:C:415:LYS:HZ2  | 1:C:448:LEU:HA   | 1.79                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:429:GLY:HA2  | 1:C:465:ASN:ND2  | 2.29                     | 0.48              |
| 1:D:105:ASP:CG   | 1:D:139:THR:HG23 | 2.33                     | 0.48              |
| 1:D:384:SER:HA   | 1:D:388:VAL:CG2  | 2.43                     | 0.48              |
| 1:D:690:ALA:CB   | 1:D:721:ILE:HG23 | 2.43                     | 0.48              |
| 1:F:579:PRO:O    | 1:F:582:VAL:HG23 | 2.14                     | 0.48              |
| 1:F:595:VAL:O    | 1:F:598:GLN:HB3  | 2.14                     | 0.48              |
| 1:A:445:ARG:HH22 | 1:A:477:LEU:CD2  | 2.27                     | 0.48              |
| 1:A:613:ARG:NE   | 1:A:613:ARG:HA   | 2.28                     | 0.48              |
| 1:B:146:TYR:CE1  | 1:B:177:GLU:HG2  | 2.49                     | 0.48              |
| 1:B:128:PHE:CD1  | 1:B:186:PRO:HG2  | 2.49                     | 0.48              |
| 1:C:111:ASP:HB3  | 1:C:172:ARG:HH22 | 1.79                     | 0.48              |
| 1:C:329:SER:HA   | 1:C:337:MSE:HE2  | 1.95                     | 0.48              |
| 1:C:367:ASP:HB2  | 1:C:424:TYR:HB3  | 1.94                     | 0.48              |
| 1:C:528:GLY:O    | 1:C:529:TYR:C    | 2.52                     | 0.48              |
| 1:D:190:LEU:O    | 1:D:196:GLN:HB2  | 2.13                     | 0.48              |
| 1:E:315:ILE:HG23 | 1:E:316:LEU:N    | 2.29                     | 0.48              |
| 1:E:670:LEU:HA   | 1:E:673:ILE:HG12 | 1.94                     | 0.48              |
| 1:F:191:TYR:HA   | 1:F:195:GLY:O    | 2.14                     | 0.48              |
| 1:F:312:THR:O    | 1:F:315:ILE:HG22 | 2.14                     | 0.48              |
| 1:F:534:ARG:HG2  | 1:F:535:LEU:N    | 2.28                     | 0.48              |
| 1:A:270:GLU:HB2  | 1:A:373:PHE:HE2  | 1.79                     | 0.48              |
| 1:A:255:LYS:HG3  | 1:A:317:PHE:CD2  | 2.49                     | 0.48              |
| 1:A:610:SER:O    | 1:A:614:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:666:PHE:O    | 1:A:669:ILE:HB   | 2.14                     | 0.48              |
| 1:B:140:ILE:HB   | 1:B:152:THR:CG2  | 2.44                     | 0.48              |
| 1:B:341:ASN:O    | 1:B:344:ALA:HB3  | 2.13                     | 0.48              |
| 1:B:595:VAL:HG12 | 1:B:595:VAL:O    | 2.13                     | 0.48              |
| 1:C:215:ILE:HD11 | 1:C:351:VAL:O    | 2.14                     | 0.48              |
| 1:C:31:ARG:HA    | 1:C:87:TYR:HB2   | 1.96                     | 0.48              |
| 1:C:406:GLU:HB3  | 1:C:464:TYR:CG   | 2.48                     | 0.48              |
| 1:C:728:VAL:C    | 1:C:730:GLU:H    | 2.17                     | 0.48              |
| 1:D:151:THR:O    | 1:D:154:LYS:HB2  | 2.13                     | 0.48              |
| 1:D:339:LYS:HD2  | 1:D:362:ILE:O    | 2.14                     | 0.48              |
| 1:D:373:PHE:CE2  | 1:D:378:ARG:HD3  | 2.48                     | 0.48              |
| 1:D:381:ILE:HA   | 1:D:717:TYR:OH   | 2.13                     | 0.48              |
| 1:D:648:ASP:OD1  | 1:D:687:LEU:HD12 | 2.14                     | 0.48              |
| 1:E:591:GLU:O    | 1:E:594:VAL:HB   | 2.14                     | 0.48              |
| 1:E:64:LYS:CB    | 1:E:65:PRO:HD2   | 2.43                     | 0.48              |
| 1:E:665:LEU:O    | 1:E:669:ILE:HG13 | 2.14                     | 0.48              |
| 1:E:751:VAL:HG13 | 1:E:752:GLY:N    | 2.29                     | 0.48              |
| 1:F:108:ILE:HG22 | 1:F:109:CYS:O    | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:495:MSE:HB3  | 1:F:500:LEU:HD11 | 1.96                     | 0.48              |
| 1:A:485:GLN:HB3  | 1:A:488:TYR:HB2  | 1.94                     | 0.48              |
| 1:B:171:ASN:HD21 | 1:B:173:ARG:CB   | 2.26                     | 0.48              |
| 1:B:335:MSE:HE2  | 1:B:335:MSE:N    | 2.29                     | 0.48              |
| 1:B:409:ASN:O    | 1:B:425:ILE:HG12 | 2.14                     | 0.48              |
| 1:C:204:ARG:C    | 1:C:204:ARG:HD2  | 2.34                     | 0.48              |
| 1:C:9:GLN:HE21   | 1:C:40:ALA:C     | 2.16                     | 0.48              |
| 1:C:525:LEU:CD2  | 1:C:534:ARG:HA   | 2.44                     | 0.48              |
| 1:C:613:ARG:NE   | 1:C:613:ARG:HA   | 2.28                     | 0.48              |
| 1:D:233:GLU:O    | 1:D:236:VAL:HG12 | 2.14                     | 0.48              |
| 1:D:255:LYS:HG2  | 1:D:256:ASP:OD2  | 2.13                     | 0.48              |
| 1:D:469:LEU:O    | 1:D:473:MSE:HB2  | 2.14                     | 0.48              |
| 1:D:496:ALA:HB2  | 1:D:755:PHE:CD2  | 2.49                     | 0.48              |
| 1:D:617:ALA:O    | 1:D:621:LEU:HB2  | 2.14                     | 0.48              |
| 1:E:130:VAL:HG22 | 1:E:131:CYS:O    | 2.14                     | 0.48              |
| 1:E:391:PRO:C    | 1:E:392:ILE:HD12 | 2.34                     | 0.48              |
| 1:E:485:GLN:HG2  | 1:E:488:TYR:CD2  | 2.49                     | 0.48              |
| 1:E:538:ILE:HG12 | 1:E:662:VAL:HG21 | 1.94                     | 0.48              |
| 1:E:624:VAL:CG1  | 1:E:637:LYS:HB3  | 2.44                     | 0.48              |
| 1:F:113:LEU:O    | 1:F:117:PHE:HB2  | 2.13                     | 0.48              |
| 1:C:127:PRO:HG3  | 1:C:203:LEU:HD21 | 1.96                     | 0.48              |
| 1:C:506:ILE:HG22 | 1:C:508:LEU:HG   | 1.95                     | 0.48              |
| 1:D:263:PHE:HD1  | 1:D:292:LEU:HD23 | 1.79                     | 0.48              |
| 1:D:218:ILE:HD12 | 1:D:356:LEU:HD23 | 1.96                     | 0.48              |
| 1:D:403:VAL:CG1  | 1:D:466:THR:HB   | 2.44                     | 0.48              |
| 1:D:470:ALA:HB1  | 1:D:481:LEU:HD11 | 1.96                     | 0.48              |
| 1:D:524:VAL:HG23 | 1:D:535:LEU:HB2  | 1.96                     | 0.48              |
| 1:E:323:PRO:HG2  | 1:E:324:VAL:H    | 1.79                     | 0.48              |
| 1:E:455:LEU:HA   | 1:E:479:VAL:HG12 | 1.95                     | 0.48              |
| 1:E:17:PHE:HZ    | 1:E:60:LEU:HD21  | 1.77                     | 0.48              |
| 1:F:16:GLY:HA2   | 1:F:132:THR:OG1  | 2.13                     | 0.48              |
| 1:F:16:GLY:O     | 1:F:19:PRO:HD2   | 2.14                     | 0.48              |
| 1:F:690:ALA:O    | 1:F:725:ILE:HG12 | 2.13                     | 0.48              |
| 1:A:573:VAL:HG13 | 1:A:574:ILE:N    | 2.29                     | 0.47              |
| 1:C:149:GLU:HB2  | 1:C:154:LYS:HZ3  | 1.78                     | 0.47              |
| 1:C:275:THR:HA   | 1:C:279:ARG:HE   | 1.79                     | 0.47              |
| 1:C:589:LYS:HG3  | 1:F:475:ASN:OD1  | 2.14                     | 0.47              |
| 1:D:279:ARG:HG3  | 1:D:309:TYR:HB3  | 1.96                     | 0.47              |
| 1:D:381:ILE:HG22 | 1:D:717:TYR:CE1  | 2.48                     | 0.47              |
| 1:E:118:ASP:HA   | 1:E:119:PRO:HD3  | 1.72                     | 0.47              |
| 1:E:177:GLU:HB2  | 1:E:178:PRO:HD3  | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:228:CYS:SG   | 1:E:229:ASP:N    | 2.87                     | 0.47              |
| 1:E:595:VAL:HG12 | 1:E:595:VAL:O    | 2.13                     | 0.47              |
| 1:F:264:ALA:HB1  | 1:F:286:LYS:HA   | 1.94                     | 0.47              |
| 1:F:380:VAL:CG1  | 1:F:381:ILE:N    | 2.77                     | 0.47              |
| 1:F:460:LEU:HB2  | 1:F:485:GLN:HA   | 1.96                     | 0.47              |
| 1:F:50:GLU:O     | 1:F:53:ILE:HG22  | 2.15                     | 0.47              |
| 1:A:18:ARG:HB2   | 1:A:19:PRO:HD3   | 1.96                     | 0.47              |
| 1:A:204:ARG:HG2  | 1:A:319:TRP:CZ2  | 2.48                     | 0.47              |
| 1:A:520:TRP:HA   | 1:A:609:SER:OG   | 2.14                     | 0.47              |
| 1:A:534:ARG:HG2  | 1:A:535:LEU:H    | 1.76                     | 0.47              |
| 1:B:204:ARG:HG3  | 1:B:319:TRP:CE2  | 2.49                     | 0.47              |
| 1:B:424:TYR:CZ   | 1:B:426:GLY:HA2  | 2.50                     | 0.47              |
| 1:B:487:HIS:CE1  | 1:B:512:GLY:HA3  | 2.49                     | 0.47              |
| 1:C:357:LEU:HD23 | 1:C:357:LEU:N    | 2.29                     | 0.47              |
| 1:C:387:PHE:O    | 1:C:390:LEU:HG   | 2.14                     | 0.47              |
| 1:C:567:ILE:HG23 | 1:C:600:ALA:HB2  | 1.95                     | 0.47              |
| 1:C:380:VAL:HG23 | 1:C:740:THR:HA   | 1.96                     | 0.47              |
| 1:D:270:GLU:CB   | 1:D:373:PHE:HE2  | 2.26                     | 0.47              |
| 1:D:709:VAL:O    | 1:D:735:ASN:HB2  | 2.14                     | 0.47              |
| 1:E:651:PHE:HB2  | 1:E:688:ALA:HB2  | 1.95                     | 0.47              |
| 1:F:301:HIS:CD2  | 1:F:302:THR:HG23 | 2.49                     | 0.47              |
| 1:F:453:LEU:O    | 1:F:453:LEU:HG   | 2.14                     | 0.47              |
| 1:F:485:GLN:HG3  | 1:F:486:HIS:N    | 2.29                     | 0.47              |
| 1:F:487:HIS:CD2  | 1:F:520:TRP:HB3  | 2.49                     | 0.47              |
| 1:F:407:LEU:HB3  | 1:F:631:GLU:OE1  | 2.14                     | 0.47              |
| 1:F:662:VAL:O    | 1:F:662:VAL:HG12 | 2.13                     | 0.47              |
| 1:A:247:GLN:HG3  | 1:A:298:PRO:CG   | 2.44                     | 0.47              |
| 1:A:422:SER:HA   | 1:A:444:PHE:CZ   | 2.49                     | 0.47              |
| 1:A:505:GLY:HA2  | 1:A:710:ALA:H    | 1.77                     | 0.47              |
| 1:A:589:LYS:N    | 1:B:475:ASN:ND2  | 2.60                     | 0.47              |
| 1:A:596:LEU:HD23 | 1:A:596:LEU:O    | 2.14                     | 0.47              |
| 1:B:189:ARG:HA   | 1:B:202:PRO:HG3  | 1.97                     | 0.47              |
| 1:B:261:LYS:NZ   | 1:B:266:VAL:HB   | 2.29                     | 0.47              |
| 1:B:526:TYR:CB   | 1:B:535:LEU:HD11 | 2.44                     | 0.47              |
| 1:B:553:PRO:HB2  | 1:B:620:VAL:CG2  | 2.45                     | 0.47              |
| 1:B:496:ALA:HB2  | 1:B:755:PHE:CD2  | 2.49                     | 0.47              |
| 1:B:756:LEU:HD21 | 1:B:770:LEU:HD22 | 1.96                     | 0.47              |
| 1:C:370:VAL:HG23 | 1:C:382:ARG:HB2  | 1.96                     | 0.47              |
| 1:C:487:HIS:HD2  | 1:C:520:TRP:HB3  | 1.79                     | 0.47              |
| 1:D:394:ILE:HD12 | 1:D:755:PHE:HB2  | 1.96                     | 0.47              |
| 1:D:485:GLN:HB3  | 1:D:488:TYR:HB2  | 1.95                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:495:MSE:SE   | 1:D:527:LEU:HD13 | 2.64                     | 0.47              |
| 1:D:554:LEU:HD21 | 1:D:579:PRO:CG   | 2.44                     | 0.47              |
| 1:D:629:HIS:HB2  | 1:D:633:GLU:OE1  | 2.14                     | 0.47              |
| 1:D:702:ARG:NH2  | 1:D:731:ALA:O    | 2.48                     | 0.47              |
| 1:E:183:VAL:HG23 | 1:E:184:CYS:H    | 1.76                     | 0.47              |
| 1:E:210:ILE:CD1  | 1:E:216:VAL:HG12 | 2.38                     | 0.47              |
| 1:E:8:VAL:HA     | 1:E:72:ARG:O     | 2.14                     | 0.47              |
| 1:F:406:GLU:HG3  | 1:F:407:LEU:H    | 1.80                     | 0.47              |
| 1:A:106:ILE:HG22 | 1:A:107:ALA:N    | 2.29                     | 0.47              |
| 1:A:154:LYS:O    | 1:A:154:LYS:HD3  | 2.14                     | 0.47              |
| 1:A:487:HIS:CE1  | 1:A:509:ASP:HB3  | 2.50                     | 0.47              |
| 1:A:516:ASP:O    | 1:A:517:GLY:C    | 2.53                     | 0.47              |
| 1:B:219:LYS:HA   | 1:B:224:ILE:CB   | 2.45                     | 0.47              |
| 1:B:310:ALA:O    | 1:B:313:HIS:HB2  | 2.14                     | 0.47              |
| 1:B:573:VAL:HG13 | 1:B:574:ILE:N    | 2.30                     | 0.47              |
| 1:B:588:GLY:O    | 1:B:592:PHE:HB2  | 2.15                     | 0.47              |
| 1:C:216:VAL:HG23 | 1:C:354:TYR:C    | 2.34                     | 0.47              |
| 1:C:309:TYR:H    | 1:C:313:HIS:CD2  | 2.32                     | 0.47              |
| 1:C:229:ASP:OD1  | 1:C:322:THR:HG21 | 2.14                     | 0.47              |
| 1:C:570:LEU:HD12 | 1:C:573:VAL:HG11 | 1.96                     | 0.47              |
| 1:C:715:VAL:HG12 | 1:C:715:VAL:O    | 2.15                     | 0.47              |
| 1:D:219:LYS:NZ   | 1:D:362:ILE:HG12 | 2.30                     | 0.47              |
| 1:E:124:TYR:CD2  | 1:E:125:MSE:HG2  | 2.49                     | 0.47              |
| 1:E:181:CYS:SG   | 1:E:182:PRO:HD2  | 2.54                     | 0.47              |
| 1:E:270:GLU:N    | 1:E:378:ARG:NH1  | 2.62                     | 0.47              |
| 1:E:579:PRO:HB3  | 1:E:626:TYR:CE1  | 2.49                     | 0.47              |
| 1:E:682:ALA:O    | 1:E:686:HIS:HB2  | 2.15                     | 0.47              |
| 1:E:727:LYS:O    | 1:E:730:GLU:HG2  | 2.15                     | 0.47              |
| 1:E:726:ARG:HG2  | 1:E:735:ASN:HD21 | 1.80                     | 0.47              |
| 1:F:264:ALA:HB1  | 1:F:285:ARG:O    | 2.15                     | 0.47              |
| 1:F:488:TYR:CD1  | 1:F:525:LEU:HD13 | 2.49                     | 0.47              |
| 1:A:218:ILE:O    | 1:A:224:ILE:HB   | 2.15                     | 0.47              |
| 1:A:406:GLU:HA   | 1:A:466:THR:HG21 | 1.95                     | 0.47              |
| 1:A:450:VAL:HG22 | 1:A:451:LYS:H    | 1.79                     | 0.47              |
| 1:A:460:LEU:HD12 | 1:A:483:GLN:HB3  | 1.97                     | 0.47              |
| 1:A:566:SER:N    | 1:A:569:GLU:HB3  | 2.28                     | 0.47              |
| 1:B:21:VAL:HG11  | 1:B:44:ILE:HD13  | 1.96                     | 0.47              |
| 1:B:457:ILE:HG22 | 1:B:458:ALA:H    | 1.78                     | 0.47              |
| 1:B:404:GLY:HA2  | 1:B:753:GLN:HE22 | 1.78                     | 0.47              |
| 1:C:111:ASP:HB3  | 1:C:172:ARG:HH12 | 1.79                     | 0.47              |
| 1:C:176:ALA:C    | 1:C:178:PRO:HD2  | 2.34                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:190:LEU:HB2  | 1:D:202:PRO:CB   | 2.41                     | 0.47              |
| 1:D:498:LYS:HE3  | 1:D:736:PHE:HB3  | 1.95                     | 0.47              |
| 1:D:642:ALA:O    | 1:D:683:TYR:HB2  | 2.14                     | 0.47              |
| 1:E:399:ASN:O    | 1:E:452:ASN:HB2  | 2.14                     | 0.47              |
| 1:F:183:VAL:CG2  | 1:F:184:CYS:N    | 2.77                     | 0.47              |
| 1:A:267:SER:HB2  | 1:A:270:GLU:HB3  | 1.94                     | 0.47              |
| 1:A:302:THR:HG21 | 1:A:372:ARG:HE   | 1.78                     | 0.47              |
| 1:B:142:GLU:HB3  | 1:B:150:ASN:O    | 2.15                     | 0.47              |
| 1:B:253:MSE:SE   | 1:B:313:HIS:ND1  | 2.97                     | 0.47              |
| 1:C:356:LEU:C    | 1:C:357:LEU:HD23 | 2.35                     | 0.47              |
| 1:C:104:PRO:HG3  | 1:C:390:LEU:HD11 | 1.95                     | 0.47              |
| 1:C:8:VAL:HG13   | 1:C:72:ARG:O     | 2.15                     | 0.47              |
| 1:D:183:VAL:CG2  | 1:D:184:CYS:N    | 2.78                     | 0.47              |
| 1:D:246:PRO:CG   | 1:D:629:HIS:HB3  | 2.45                     | 0.47              |
| 1:D:535:LEU:HD23 | 1:D:700:ARG:HG3  | 1.95                     | 0.47              |
| 1:E:373:PHE:CE2  | 1:E:378:ARG:HD3  | 2.49                     | 0.47              |
| 1:E:398:TYR:HB2  | 1:E:454:ASP:CG   | 2.35                     | 0.47              |
| 1:E:413:VAL:HG21 | 1:E:448:LEU:HD13 | 1.95                     | 0.47              |
| 1:E:553:PRO:HB2  | 1:E:620:VAL:CG2  | 2.41                     | 0.47              |
| 1:E:665:LEU:HG   | 1:E:669:ILE:HD11 | 1.97                     | 0.47              |
| 1:F:250:PHE:HE2  | 1:F:328:THR:OG1  | 1.96                     | 0.47              |
| 1:A:582:VAL:HG13 | 1:A:626:TYR:HB3  | 1.95                     | 0.47              |
| 1:A:677:SER:HB2  | 1:A:678:PRO:HD2  | 1.97                     | 0.47              |
| 1:B:370:VAL:CG2  | 1:B:381:ILE:HD11 | 2.44                     | 0.47              |
| 1:C:286:LYS:HE3  | 1:C:290:PHE:CA   | 2.43                     | 0.47              |
| 1:C:523:GLU:CD   | 1:C:523:GLU:N    | 2.68                     | 0.47              |
| 1:C:543:LEU:HD23 | 1:C:543:LEU:N    | 2.18                     | 0.47              |
| 1:C:760:TYR:HE2  | 1:C:767:LYS:HG2  | 1.80                     | 0.47              |
| 1:D:251:ALA:HB3  | 1:D:327:MSE:O    | 2.14                     | 0.47              |
| 1:D:13:GLN:HG3   | 1:D:42:VAL:HG23  | 1.97                     | 0.47              |
| 1:D:403:VAL:HG23 | 1:D:457:ILE:O    | 2.15                     | 0.47              |
| 1:D:504:ILE:HG22 | 1:D:505:GLY:H    | 1.79                     | 0.47              |
| 1:E:252:ILE:HD13 | 1:E:303:ILE:CG2  | 2.45                     | 0.47              |
| 1:F:374:VAL:HG21 | 1:F:744:ARG:CZ   | 2.45                     | 0.47              |
| 1:F:504:ILE:HG23 | 1:F:525:LEU:O    | 2.15                     | 0.47              |
| 1:F:694:ALA:C    | 1:F:696:THR:N    | 2.68                     | 0.47              |
| 1:A:264:ALA:HB1  | 1:A:285:ARG:O    | 2.15                     | 0.47              |
| 1:A:660:ILE:O    | 1:A:662:VAL:HG23 | 2.14                     | 0.47              |
| 1:B:168:ASP:O    | 1:B:174:TYR:HB2  | 2.15                     | 0.47              |
| 1:C:729:VAL:HB   | 1:C:735:ASN:HD22 | 1.78                     | 0.47              |
| 1:D:130:VAL:HG21 | 1:D:135:GLY:HA3  | 1.96                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:111:ASP:CB   | 1:D:172:ARG:HH12 | 2.17                     | 0.47              |
| 1:D:1:MSE:HE3    | 1:D:84:ASP:N     | 2.30                     | 0.47              |
| 1:D:286:LYS:HB2  | 1:D:303:ILE:CD1  | 2.45                     | 0.47              |
| 1:D:451:LYS:HD3  | 1:D:477:LEU:CG   | 2.45                     | 0.47              |
| 1:E:134:CYS:SG   | 1:E:135:GLY:N    | 2.87                     | 0.47              |
| 1:E:166:TYR:CE1  | 1:E:175:HIS:HA   | 2.50                     | 0.47              |
| 1:E:266:VAL:HG22 | 1:E:284:LEU:HD13 | 1.97                     | 0.47              |
| 1:F:300:LEU:CD2  | 1:F:636:MSE:HE2  | 2.45                     | 0.47              |
| 1:F:283:THR:OG1  | 1:F:372:ARG:HB2  | 2.15                     | 0.47              |
| 1:F:408:MSE:HG3  | 1:F:424:TYR:HE1  | 1.78                     | 0.47              |
| 1:A:128:PHE:CD1  | 1:A:186:PRO:HG2  | 2.50                     | 0.47              |
| 1:A:129:ILE:O    | 1:A:130:VAL:HB   | 2.15                     | 0.47              |
| 1:A:253:MSE:HE2  | 1:A:317:PHE:HD1  | 1.79                     | 0.47              |
| 1:A:1:MSE:HB2    | 1:A:80:PRO:HD2   | 1.96                     | 0.47              |
| 1:B:739:THR:O    | 1:B:742:VAL:O    | 2.33                     | 0.47              |
| 1:C:451:LYS:HA   | 1:C:477:LEU:HD21 | 1.95                     | 0.47              |
| 1:D:126:TYR:CD1  | 1:D:182:PRO:HG3  | 2.50                     | 0.47              |
| 1:D:257:ILE:HA   | 1:D:260:VAL:HG23 | 1.96                     | 0.47              |
| 1:E:193:SER:O    | 1:E:194:ASP:CB   | 2.59                     | 0.47              |
| 1:E:190:LEU:O    | 1:E:196:GLN:HB2  | 2.15                     | 0.47              |
| 1:E:245:ARG:NE   | 1:E:248:LYS:HB3  | 2.30                     | 0.47              |
| 1:E:370:VAL:HG23 | 1:E:381:ILE:CG1  | 2.45                     | 0.47              |
| 1:E:406:GLU:HB3  | 1:E:464:TYR:CG   | 2.50                     | 0.47              |
| 1:F:306:MSE:O    | 1:F:307:LEU:HD23 | 2.15                     | 0.47              |
| 1:F:509:ASP:CG   | 1:F:510:GLY:H    | 2.18                     | 0.47              |
| 1:F:595:VAL:O    | 1:F:595:VAL:HG12 | 2.15                     | 0.47              |
| 1:F:726:ARG:HH21 | 1:F:727:LYS:HG2  | 1.76                     | 0.47              |
| 1:F:766:THR:OG1  | 1:F:769:ASP:HB2  | 2.14                     | 0.47              |
| 1:A:131:CYS:SG   | 1:A:133:ASN:HB2  | 2.54                     | 0.47              |
| 1:A:252:ILE:HG22 | 1:A:253:MSE:N    | 2.30                     | 0.47              |
| 1:A:315:ILE:HG23 | 1:A:316:LEU:N    | 2.30                     | 0.47              |
| 1:A:283:THR:OG1  | 1:A:372:ARG:HB2  | 2.15                     | 0.47              |
| 1:A:515:THR:O    | 1:A:516:ASP:HB2  | 2.14                     | 0.47              |
| 1:B:284:LEU:O    | 1:B:302:THR:HA   | 2.14                     | 0.47              |
| 1:C:147:ASP:HA   | 1:C:177:GLU:OE2  | 2.15                     | 0.47              |
| 1:C:210:ILE:HD11 | 1:C:228:CYS:N    | 2.30                     | 0.47              |
| 1:C:35:LYS:HG2   | 1:C:36:ASN:H     | 1.80                     | 0.47              |
| 1:C:456:ILE:HD11 | 1:C:479:VAL:HB   | 1.96                     | 0.47              |
| 1:D:278:ARG:HG3  | 1:D:280:PRO:HD3  | 1.95                     | 0.47              |
| 1:D:320:SER:HG   | 1:D:325:TYR:HE1  | 1.61                     | 0.47              |
| 1:E:144:LEU:HA   | 1:E:145:PRO:C    | 2.36                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:204:ARG:HD2  | 1:E:204:ARG:C    | 2.36                     | 0.47              |
| 1:E:566:SER:HB3  | 1:E:569:GLU:HG2  | 1.97                     | 0.47              |
| 1:F:286:LYS:CE   | 1:F:290:PHE:HB2  | 2.45                     | 0.47              |
| 1:F:404:GLY:O    | 1:F:459:ASP:HB2  | 2.15                     | 0.47              |
| 1:C:590:VAL:HG23 | 1:F:475:ASN:OD1  | 2.14                     | 0.47              |
| 1:F:404:GLY:HA2  | 1:F:753:GLN:CD   | 2.35                     | 0.47              |
| 1:A:719:GLU:O    | 1:A:723:LYS:HB2  | 2.14                     | 0.47              |
| 1:A:412:GLY:CA   | 1:A:750:ASN:HD22 | 2.22                     | 0.47              |
| 1:B:566:SER:H    | 1:B:569:GLU:CB   | 2.28                     | 0.47              |
| 1:B:665:LEU:O    | 1:B:669:ILE:HG13 | 2.15                     | 0.47              |
| 1:B:6:ILE:HG22   | 1:B:7:HIS:H      | 1.80                     | 0.47              |
| 1:C:66:PRO:CG    | 1:C:133:ASN:HB3  | 2.44                     | 0.47              |
| 1:C:251:ALA:HB3  | 1:C:327:MSE:O    | 2.14                     | 0.47              |
| 1:C:219:LYS:HZ2  | 1:C:362:ILE:HG12 | 1.80                     | 0.47              |
| 1:C:625:ALA:HB2  | 1:C:637:LYS:CD   | 2.44                     | 0.47              |
| 1:C:718:ASN:ND2  | 1:C:720:LEU:HB2  | 2.30                     | 0.47              |
| 1:D:219:LYS:HA   | 1:D:224:ILE:CB   | 2.45                     | 0.47              |
| 1:D:540:TYR:O    | 1:D:563:LYS:HE3  | 2.15                     | 0.47              |
| 1:D:17:PHE:CZ    | 1:D:60:LEU:HD11  | 2.50                     | 0.47              |
| 1:D:66:PRO:HG2   | 1:D:67:LEU:H     | 1.80                     | 0.47              |
| 1:E:383:ARG:HH11 | 1:E:383:ARG:HG3  | 1.80                     | 0.47              |
| 1:E:486:HIS:O    | 1:E:489:ALA:HB3  | 2.14                     | 0.47              |
| 1:A:323:PRO:HG2  | 1:A:324:VAL:H    | 1.79                     | 0.46              |
| 1:B:651:PHE:HB2  | 1:B:688:ALA:HB2  | 1.97                     | 0.46              |
| 1:C:172:ARG:HG2  | 1:C:173:ARG:N    | 2.30                     | 0.46              |
| 1:C:274:LEU:O    | 1:C:307:LEU:HD12 | 2.15                     | 0.46              |
| 1:C:427:ASN:ND2  | 1:C:429:GLY:H    | 2.12                     | 0.46              |
| 1:C:415:LYS:NZ   | 1:C:448:LEU:HA   | 2.30                     | 0.46              |
| 1:C:558:MSE:HE1  | 1:C:593:ASN:OD1  | 2.15                     | 0.46              |
| 1:D:288:GLU:CB   | 1:D:289:PRO:HD3  | 2.30                     | 0.46              |
| 1:D:299:GLY:O    | 1:D:300:LEU:HG   | 2.15                     | 0.46              |
| 1:D:371:ILE:HD11 | 1:D:373:PHE:HE1  | 1.80                     | 0.46              |
| 1:D:409:ASN:HD22 | 1:D:437:MSE:HE2  | 1.80                     | 0.46              |
| 1:D:589:LYS:HG3  | 1:D:590:VAL:N    | 2.25                     | 0.46              |
| 1:D:742:VAL:CG1  | 1:D:751:VAL:HG11 | 2.45                     | 0.46              |
| 1:E:216:VAL:O    | 1:E:227:ALA:HB3  | 2.15                     | 0.46              |
| 1:E:287:LYS:O    | 1:E:288:GLU:C    | 2.53                     | 0.46              |
| 1:E:485:GLN:NE2  | 1:E:486:HIS:H    | 2.13                     | 0.46              |
| 1:F:1:MSE:CB     | 1:F:80:PRO:HD2   | 2.46                     | 0.46              |
| 1:F:213:GLY:C    | 1:F:235:VAL:HG11 | 2.35                     | 0.46              |
| 1:F:30:LEU:O     | 1:F:30:LEU:HD23  | 2.14                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:445:ARG:HH21 | 1:F:452:ASN:ND2  | 2.13                     | 0.46              |
| 1:F:472:GLU:HG3  | 1:F:473:MSE:N    | 2.30                     | 0.46              |
| 1:A:400:GLY:O    | 1:A:413:VAL:HG23 | 2.15                     | 0.46              |
| 1:A:403:VAL:CG1  | 1:A:466:THR:HB   | 2.45                     | 0.46              |
| 1:B:137:ARG:O    | 1:B:141:ILE:HG13 | 2.15                     | 0.46              |
| 1:B:1:MSE:HE3    | 1:B:2:LYS:H      | 1.79                     | 0.46              |
| 1:B:254:ALA:HB1  | 1:B:259:THR:CB   | 2.41                     | 0.46              |
| 1:C:572:GLY:HA2  | 1:C:575:ASN:HD22 | 1.80                     | 0.46              |
| 1:D:678:PRO:HG2  | 1:D:679:ALA:H    | 1.80                     | 0.46              |
| 1:D:398:TYR:CE1  | 1:D:758:GLY:HA3  | 2.50                     | 0.46              |
| 1:E:443:HIS:O    | 1:E:447:ILE:HD12 | 2.15                     | 0.46              |
| 1:E:694:ALA:HB2  | 1:E:725:ILE:HG23 | 1.96                     | 0.46              |
| 1:F:394:ILE:HG22 | 1:F:396:PHE:H    | 1.81                     | 0.46              |
| 1:F:456:ILE:HD11 | 1:F:479:VAL:HB   | 1.98                     | 0.46              |
| 1:F:584:SER:CB   | 1:F:589:LYS:HB3  | 2.46                     | 0.46              |
| 1:F:507:ALA:HA   | 1:F:712:SER:O    | 2.16                     | 0.46              |
| 1:A:123:ARG:HE   | 1:A:173:ARG:HH21 | 1.62                     | 0.46              |
| 1:A:88:ILE:HG22  | 1:A:89:GLU:N     | 2.30                     | 0.46              |
| 1:B:154:LYS:HD3  | 1:B:154:LYS:C    | 2.36                     | 0.46              |
| 1:B:217:ALA:O    | 1:B:218:ILE:HD13 | 2.16                     | 0.46              |
| 1:B:365:ARG:O    | 1:B:423:GLN:HG2  | 2.16                     | 0.46              |
| 1:B:437:MSE:HG2  | 1:B:441:ILE:HD11 | 1.97                     | 0.46              |
| 1:B:491:ILE:CD1  | 1:B:525:LEU:HD12 | 2.45                     | 0.46              |
| 1:C:323:PRO:HG2  | 1:C:324:VAL:H    | 1.80                     | 0.46              |
| 1:C:550:SER:O    | 1:C:628:ARG:HD2  | 2.14                     | 0.46              |
| 1:D:158:MSE:HE1  | 1:D:166:TYR:CD2  | 2.49                     | 0.46              |
| 1:D:455:LEU:HA   | 1:D:479:VAL:HG12 | 1.97                     | 0.46              |
| 1:D:472:GLU:HG3  | 1:D:473:MSE:N    | 2.30                     | 0.46              |
| 1:E:343:ARG:HH11 | 1:E:343:ARG:HG2  | 1.81                     | 0.46              |
| 1:F:282:ILE:HA   | 1:F:371:ILE:O    | 2.15                     | 0.46              |
| 1:A:690:ALA:CB   | 1:A:721:ILE:HG23 | 2.46                     | 0.46              |
| 1:B:376:GLY:O    | 1:B:377:LYS:HG3  | 2.15                     | 0.46              |
| 1:B:428:THR:HG21 | 1:B:437:MSE:HE1  | 1.96                     | 0.46              |
| 1:B:582:VAL:CG1  | 1:B:626:TYR:HB3  | 2.46                     | 0.46              |
| 1:B:584:SER:CB   | 1:B:589:LYS:HB3  | 2.44                     | 0.46              |
| 1:B:707:LYS:HG3  | 1:B:708:ASN:CG   | 2.36                     | 0.46              |
| 1:C:213:GLY:C    | 1:C:235:VAL:HG11 | 2.35                     | 0.46              |
| 1:C:409:ASN:HB3  | 1:C:425:ILE:HD11 | 1.97                     | 0.46              |
| 1:C:486:HIS:O    | 1:C:489:ALA:HB3  | 2.16                     | 0.46              |
| 1:C:65:PRO:C     | 1:C:67:LEU:H     | 2.17                     | 0.46              |
| 1:C:8:VAL:HG22   | 1:C:72:ARG:O     | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:18:ARG:O     | 1:D:21:VAL:HG12  | 2.16                     | 0.46              |
| 1:D:270:GLU:HB2  | 1:D:373:PHE:CE2  | 2.48                     | 0.46              |
| 1:D:268:PRO:C    | 1:D:270:GLU:H    | 2.18                     | 0.46              |
| 1:D:370:VAL:HG23 | 1:D:381:ILE:HG13 | 1.97                     | 0.46              |
| 1:E:124:TYR:CE2  | 1:E:125:MSE:HG2  | 2.50                     | 0.46              |
| 1:F:16:GLY:HA3   | 1:F:132:THR:O    | 2.15                     | 0.46              |
| 1:F:279:ARG:HG3  | 1:F:309:TYR:HB3  | 1.96                     | 0.46              |
| 1:F:335:MSE:HE2  | 1:F:335:MSE:N    | 2.30                     | 0.46              |
| 1:F:495:MSE:HG3  | 1:F:755:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:18:ARG:HG3   | 1:A:18:ARG:NH1   | 2.30                     | 0.46              |
| 1:B:269:GLU:HB2  | 1:B:378:ARG:NH2  | 2.31                     | 0.46              |
| 1:B:398:TYR:O    | 1:B:398:TYR:CG   | 2.69                     | 0.46              |
| 1:B:406:GLU:HG3  | 1:B:407:LEU:HG   | 1.97                     | 0.46              |
| 1:B:555:ARG:NH2  | 1:B:595:VAL:HG11 | 2.31                     | 0.46              |
| 1:B:522:GLY:CA   | 1:B:611:THR:HG23 | 2.46                     | 0.46              |
| 1:C:330:ALA:HB1  | 1:C:348:LEU:HD21 | 1.96                     | 0.46              |
| 1:D:123:ARG:HD3  | 1:D:129:ILE:HG13 | 1.98                     | 0.46              |
| 1:D:225:HIS:HA   | 1:D:330:ALA:H    | 1.80                     | 0.46              |
| 1:D:433:VAL:O    | 1:D:436:PHE:HB3  | 2.15                     | 0.46              |
| 1:E:312:THR:HA   | 1:E:315:ILE:CG2  | 2.45                     | 0.46              |
| 1:E:88:ILE:HD12  | 1:E:88:ILE:N     | 2.30                     | 0.46              |
| 1:F:203:LEU:HD12 | 1:F:319:TRP:CZ3  | 2.46                     | 0.46              |
| 1:F:380:VAL:HG12 | 1:F:381:ILE:H    | 1.78                     | 0.46              |
| 1:F:380:VAL:HG23 | 1:F:740:THR:CA   | 2.39                     | 0.46              |
| 1:F:374:VAL:HG21 | 1:F:744:ARG:NH1  | 2.30                     | 0.46              |
| 1:A:210:ILE:O    | 1:A:229:ASP:HB2  | 2.15                     | 0.46              |
| 1:A:540:TYR:HA   | 1:A:608:ALA:O    | 2.15                     | 0.46              |
| 1:A:542:PRO:O    | 1:A:559:GLY:CA   | 2.61                     | 0.46              |
| 1:A:616:ASP:O    | 1:A:619:ALA:HB3  | 2.15                     | 0.46              |
| 1:A:582:VAL:HG11 | 1:A:626:TYR:HB3  | 1.97                     | 0.46              |
| 1:B:165:GLU:HB3  | 1:B:171:ASN:CG   | 2.36                     | 0.46              |
| 1:B:371:ILE:CD1  | 1:B:380:VAL:HG22 | 2.42                     | 0.46              |
| 1:B:24:ILE:HG23  | 1:B:56:PHE:CE1   | 2.50                     | 0.46              |
| 1:B:651:PHE:HB2  | 1:B:688:ALA:CB   | 2.46                     | 0.46              |
| 1:C:331:ASN:ND2  | 1:C:337:MSE:HA   | 2.20                     | 0.46              |
| 1:C:273:GLU:CG   | 1:C:371:ILE:HD13 | 2.41                     | 0.46              |
| 1:C:522:GLY:HA2  | 1:C:611:THR:HG23 | 1.97                     | 0.46              |
| 1:D:383:ARG:H    | 1:D:747:ASN:ND2  | 2.13                     | 0.46              |
| 1:D:391:PRO:HB3  | 1:D:420:TYR:CD1  | 2.51                     | 0.46              |
| 1:D:7:HIS:CD2    | 1:D:43:GLU:HG3   | 2.51                     | 0.46              |
| 1:D:447:ILE:O    | 1:D:447:ILE:HG22 | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:32:GLY:HA3   | 1:D:45:VAL:O     | 2.15                     | 0.46              |
| 1:D:523:GLU:HG3  | 1:D:537:HIS:HB2  | 1.96                     | 0.46              |
| 1:D:584:SER:HB3  | 1:D:589:LYS:HB3  | 1.98                     | 0.46              |
| 1:D:618:ILE:O    | 1:D:622:LEU:HG   | 2.15                     | 0.46              |
| 1:E:286:LYS:HD2  | 1:E:303:ILE:CD1  | 2.45                     | 0.46              |
| 1:E:707:LYS:O    | 1:E:733:GLY:HA3  | 2.15                     | 0.46              |
| 1:E:742:VAL:HG11 | 1:E:751:VAL:HG11 | 1.98                     | 0.46              |
| 1:E:7:HIS:HB2    | 1:E:74:GLU:HB2   | 1.98                     | 0.46              |
| 1:F:278:ARG:CG   | 1:F:280:PRO:HD3  | 2.46                     | 0.46              |
| 1:A:171:ASN:ND2  | 1:A:173:ARG:HB2  | 2.30                     | 0.46              |
| 1:A:239:LEU:HD13 | 1:A:250:PHE:CE1  | 2.50                     | 0.46              |
| 1:A:239:LEU:O    | 1:A:239:LEU:HD23 | 2.16                     | 0.46              |
| 1:A:276:SER:OG   | 1:A:278:ARG:HG2  | 2.15                     | 0.46              |
| 1:A:592:PHE:O    | 1:A:595:VAL:HB   | 2.15                     | 0.46              |
| 1:B:255:LYS:HG2  | 1:B:256:ASP:OD2  | 2.16                     | 0.46              |
| 1:B:312:THR:HA   | 1:B:315:ILE:HG22 | 1.98                     | 0.46              |
| 1:C:399:ASN:N    | 1:C:399:ASN:HD22 | 2.12                     | 0.46              |
| 1:C:486:HIS:HD2  | 1:C:487:HIS:ND1  | 2.13                     | 0.46              |
| 1:C:620:VAL:C    | 1:C:622:LEU:N    | 2.68                     | 0.46              |
| 1:D:749:VAL:O    | 1:D:753:GLN:HG3  | 2.16                     | 0.46              |
| 1:D:57:ILE:HG13  | 1:D:75:LYS:HZ1   | 1.79                     | 0.46              |
| 1:E:104:PRO:HB3  | 1:E:387:PHE:O    | 2.16                     | 0.46              |
| 1:E:570:LEU:O    | 1:E:574:ILE:HG12 | 2.16                     | 0.46              |
| 1:E:589:LYS:HG3  | 1:E:590:VAL:HG23 | 1.97                     | 0.46              |
| 1:F:247:GLN:HG3  | 1:F:298:PRO:CG   | 2.41                     | 0.46              |
| 1:A:664:GLU:O    | 1:A:667:GLN:HB3  | 2.16                     | 0.46              |
| 1:A:380:VAL:CG2  | 1:A:740:THR:HG23 | 2.45                     | 0.46              |
| 1:B:181:CYS:SG   | 1:B:182:PRO:HD2  | 2.56                     | 0.46              |
| 1:B:587:TYR:CD1  | 1:B:588:GLY:N    | 2.78                     | 0.46              |
| 1:C:226:LEU:HD11 | 1:C:348:LEU:HD23 | 1.97                     | 0.46              |
| 1:C:371:ILE:CD1  | 1:C:380:VAL:HG22 | 2.36                     | 0.46              |
| 1:D:127:PRO:O    | 1:D:311:GLY:HA3  | 2.16                     | 0.46              |
| 1:D:286:LYS:HZ3  | 1:D:292:LEU:HB2  | 1.80                     | 0.46              |
| 1:D:190:LEU:HD12 | 1:D:355:PHE:O    | 2.16                     | 0.46              |
| 1:D:380:VAL:HG23 | 1:D:740:THR:CA   | 2.42                     | 0.46              |
| 1:E:16:GLY:O     | 1:E:19:PRO:HD2   | 2.16                     | 0.46              |
| 1:E:525:LEU:HA   | 1:E:535:LEU:HD13 | 1.98                     | 0.46              |
| 1:D:475:ASN:HD21 | 1:E:590:VAL:N    | 2.14                     | 0.46              |
| 1:F:144:LEU:HA   | 1:F:145:PRO:C    | 2.36                     | 0.46              |
| 1:F:218:ILE:O    | 1:F:224:ILE:HG23 | 2.16                     | 0.46              |
| 1:A:121:ASN:HD22 | 1:A:123:ARG:H    | 1.63                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:464:TYR:C    | 1:A:466:THR:H    | 2.19                     | 0.46              |
| 1:A:580:LYS:C    | 1:A:582:VAL:H    | 2.18                     | 0.46              |
| 1:A:670:LEU:HA   | 1:A:673:ILE:HG12 | 1.98                     | 0.46              |
| 1:A:759:LEU:CD2  | 1:A:764:TYR:HB2  | 2.46                     | 0.46              |
| 1:B:189:ARG:O    | 1:B:356:LEU:HA   | 2.15                     | 0.46              |
| 1:B:410:ALA:HB3  | 1:B:747:ASN:O    | 2.16                     | 0.46              |
| 1:D:114:ARG:O    | 1:D:118:ASP:HB2  | 2.16                     | 0.46              |
| 1:D:268:PRO:HG2  | 1:D:378:ARG:HH22 | 1.81                     | 0.46              |
| 1:E:335:MSE:CE   | 1:E:430:LYS:HG3  | 2.46                     | 0.46              |
| 1:E:545:GLY:HA3  | 1:E:548:LEU:HD12 | 1.98                     | 0.46              |
| 1:E:541:TYR:CG   | 1:E:560:ILE:HG22 | 2.51                     | 0.46              |
| 1:F:205:LYS:HA   | 1:F:208:GLU:HG3  | 1.98                     | 0.46              |
| 1:F:413:VAL:CG1  | 1:F:420:TYR:HB2  | 2.46                     | 0.46              |
| 1:F:460:LEU:CD2  | 1:F:515:THR:HG22 | 2.45                     | 0.46              |
| 1:F:542:PRO:HD2  | 1:F:563:LYS:HG3  | 1.98                     | 0.46              |
| 1:F:380:VAL:CG2  | 1:F:740:THR:HG23 | 2.46                     | 0.46              |
| 1:A:126:TYR:OH   | 1:A:185:GLY:HA3  | 2.15                     | 0.46              |
| 1:A:225:HIS:CD2  | 1:A:327:MSE:HB3  | 2.51                     | 0.46              |
| 1:A:365:ARG:O    | 1:A:423:GLN:HG2  | 2.16                     | 0.46              |
| 1:A:445:ARG:NH2  | 1:A:452:ASN:ND2  | 2.63                     | 0.46              |
| 1:A:543:LEU:HD23 | 1:A:606:ALA:O    | 2.16                     | 0.46              |
| 1:A:660:ILE:HG22 | 1:A:662:VAL:HG22 | 1.97                     | 0.46              |
| 1:B:205:LYS:O    | 1:B:208:GLU:HB3  | 2.16                     | 0.46              |
| 1:B:228:CYS:SG   | 1:B:235:VAL:HG23 | 2.56                     | 0.46              |
| 1:B:538:ILE:HG23 | 1:B:662:VAL:CG2  | 2.46                     | 0.46              |
| 1:C:485:GLN:CG   | 1:C:488:TYR:H    | 2.20                     | 0.46              |
| 1:C:582:VAL:HG21 | 1:C:626:TYR:HB3  | 1.97                     | 0.46              |
| 1:C:726:ARG:HH21 | 1:C:727:LYS:HA   | 1.81                     | 0.46              |
| 1:C:738:VAL:HG21 | 1:C:744:ARG:HB3  | 1.98                     | 0.46              |
| 1:D:410:ALA:HB3  | 1:D:747:ASN:O    | 2.16                     | 0.46              |
| 1:D:432:GLU:H    | 1:D:432:GLU:CD   | 2.19                     | 0.46              |
| 1:E:20:PHE:CZ    | 1:E:63:LYS:HB3   | 2.51                     | 0.46              |
| 1:E:219:LYS:HA   | 1:E:224:ILE:HB   | 1.98                     | 0.46              |
| 1:E:301:HIS:CD2  | 1:E:301:HIS:N    | 2.83                     | 0.46              |
| 1:E:369:SER:HB2  | 1:E:385:ARG:HB3  | 1.97                     | 0.46              |
| 1:F:163:ARG:HA   | 1:F:166:TYR:HB3  | 1.97                     | 0.46              |
| 1:F:191:TYR:CD1  | 1:F:196:GLN:HB3  | 2.50                     | 0.46              |
| 1:A:288:GLU:CB   | 1:A:289:PRO:HD3  | 2.34                     | 0.45              |
| 1:A:310:ALA:O    | 1:A:311:GLY:C    | 2.54                     | 0.45              |
| 1:A:651:PHE:HB2  | 1:A:688:ALA:HB2  | 1.97                     | 0.45              |
| 1:B:15:VAL:HG12  | 1:B:16:GLY:N     | 2.30                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:20:PHE:O     | 1:B:24:ILE:HG22  | 2.16                     | 0.45              |
| 1:B:25:ALA:HA    | 1:B:56:PHE:HE1   | 1.80                     | 0.45              |
| 1:B:751:VAL:HG13 | 1:B:752:GLY:H    | 1.80                     | 0.45              |
| 1:C:151:THR:O    | 1:C:154:LYS:HB2  | 2.17                     | 0.45              |
| 1:C:557:LEU:O    | 1:C:561:LEU:HG   | 2.15                     | 0.45              |
| 1:C:595:VAL:O    | 1:C:595:VAL:HG12 | 2.16                     | 0.45              |
| 1:C:649:LEU:HD12 | 1:C:650:LYS:N    | 2.31                     | 0.45              |
| 1:D:233:GLU:HA   | 1:D:236:VAL:HG12 | 1.98                     | 0.45              |
| 1:D:406:GLU:HG3  | 1:D:407:LEU:N    | 2.31                     | 0.45              |
| 1:D:88:ILE:N     | 1:D:88:ILE:HD12  | 2.30                     | 0.45              |
| 1:E:270:GLU:HB2  | 1:E:373:PHE:CE2  | 2.34                     | 0.45              |
| 1:E:738:VAL:CG2  | 1:E:744:ARG:HG2  | 2.35                     | 0.45              |
| 1:F:749:VAL:O    | 1:F:753:GLN:HG3  | 2.16                     | 0.45              |
| 1:A:383:ARG:HD2  | 1:A:387:PHE:CD2  | 2.52                     | 0.45              |
| 1:A:451:LYS:HD3  | 1:A:477:LEU:HD11 | 1.97                     | 0.45              |
| 1:A:9:GLN:NE2    | 1:A:40:ALA:HB1   | 2.31                     | 0.45              |
| 1:B:139:THR:HG21 | 1:B:222:GLY:HA3  | 1.97                     | 0.45              |
| 1:C:163:ARG:NH1  | 1:C:163:ARG:HB2  | 2.31                     | 0.45              |
| 1:C:274:LEU:HD23 | 1:C:274:LEU:HA   | 1.71                     | 0.45              |
| 1:C:485:GLN:CG   | 1:C:488:TYR:HB2  | 2.46                     | 0.45              |
| 1:C:495:MSE:HE2  | 1:C:755:PHE:HZ   | 1.81                     | 0.45              |
| 1:D:116:LEU:HG   | 1:D:117:PHE:N    | 2.32                     | 0.45              |
| 1:D:144:LEU:HA   | 1:D:145:PRO:C    | 2.37                     | 0.45              |
| 1:D:181:CYS:HG   | 1:D:183:VAL:HG22 | 1.82                     | 0.45              |
| 1:D:261:LYS:HA   | 1:D:264:ALA:O    | 2.16                     | 0.45              |
| 1:D:138:PHE:HB2  | 1:D:389:PRO:HD3  | 1.97                     | 0.45              |
| 1:E:269:GLU:HB2  | 1:E:378:ARG:NH2  | 2.32                     | 0.45              |
| 1:D:475:ASN:ND2  | 1:E:591:GLU:H    | 2.13                     | 0.45              |
| 1:E:62:LYS:O     | 1:E:63:LYS:HG3   | 2.16                     | 0.45              |
| 1:F:263:PHE:HD1  | 1:F:292:LEU:HD23 | 1.81                     | 0.45              |
| 1:F:13:GLN:HB2   | 1:F:42:VAL:HG22  | 1.98                     | 0.45              |
| 1:A:216:VAL:O    | 1:A:227:ALA:HB3  | 2.16                     | 0.45              |
| 1:A:558:MSE:HE1  | 1:A:593:ASN:OD1  | 2.16                     | 0.45              |
| 1:A:737:HIS:O    | 1:A:738:VAL:C    | 2.55                     | 0.45              |
| 1:B:743:PRO:HG3  | 1:B:747:ASN:ND2  | 2.32                     | 0.45              |
| 1:D:253:MSE:HE1  | 1:D:313:HIS:CG   | 2.51                     | 0.45              |
| 1:D:203:LEU:HD21 | 1:D:315:ILE:HG21 | 1.99                     | 0.45              |
| 1:D:370:VAL:CG2  | 1:D:381:ILE:HD11 | 2.47                     | 0.45              |
| 1:D:557:LEU:HD23 | 1:D:557:LEU:C    | 2.37                     | 0.45              |
| 1:D:752:GLY:O    | 1:D:756:LEU:HB2  | 2.16                     | 0.45              |
| 1:F:217:ALA:HA   | 1:F:226:LEU:HA   | 1.97                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:506:ILE:CD1  | 1:F:694:ALA:HA   | 2.46                     | 0.45              |
| 1:F:619:ALA:HA   | 1:F:638:LEU:HD13 | 1.97                     | 0.45              |
| 1:F:642:ALA:HB1  | 1:F:683:TYR:HA   | 1.98                     | 0.45              |
| 1:A:134:CYS:SG   | 1:A:135:GLY:N    | 2.90                     | 0.45              |
| 1:A:158:MSE:HE3  | 1:A:163:ARG:HH12 | 1.81                     | 0.45              |
| 1:A:168:ASP:O    | 1:A:174:TYR:HD2  | 2.00                     | 0.45              |
| 1:A:293:PRO:C    | 1:A:295:ASN:H    | 2.19                     | 0.45              |
| 1:A:739:THR:O    | 1:A:740:THR:C    | 2.55                     | 0.45              |
| 1:B:738:VAL:HG12 | 1:B:742:VAL:O    | 2.17                     | 0.45              |
| 1:C:140:ILE:HB   | 1:C:152:THR:CG2  | 2.46                     | 0.45              |
| 1:C:154:LYS:C    | 1:C:156:PHE:H    | 2.18                     | 0.45              |
| 1:C:239:LEU:HD22 | 1:C:250:PHE:CE1  | 2.51                     | 0.45              |
| 1:C:398:TYR:CE1  | 1:C:758:GLY:HA3  | 2.51                     | 0.45              |
| 1:C:67:LEU:HD21  | 1:C:106:ILE:HD11 | 1.98                     | 0.45              |
| 1:D:165:GLU:HB3  | 1:D:171:ASN:ND2  | 2.31                     | 0.45              |
| 1:E:15:VAL:HG12  | 1:E:16:GLY:N     | 2.31                     | 0.45              |
| 1:E:485:GLN:NE2  | 1:E:486:HIS:N    | 2.64                     | 0.45              |
| 1:F:589:LYS:HG3  | 1:F:590:VAL:HG23 | 1.98                     | 0.45              |
| 1:A:240:ARG:HB3  | 1:A:245:ARG:O    | 2.17                     | 0.45              |
| 1:A:288:GLU:HB3  | 1:A:289:PRO:CD   | 2.33                     | 0.45              |
| 1:A:320:SER:O    | 1:A:322:THR:N    | 2.50                     | 0.45              |
| 1:A:38:GLY:C     | 1:A:40:ALA:H     | 2.20                     | 0.45              |
| 1:B:265:TYR:HE2  | 1:B:287:LYS:HD2  | 1.81                     | 0.45              |
| 1:B:331:ASN:HD22 | 1:B:337:MSE:CA   | 2.23                     | 0.45              |
| 1:C:411:PHE:CZ   | 1:C:441:ILE:HA   | 2.51                     | 0.45              |
| 1:C:742:VAL:CG1  | 1:C:751:VAL:HG11 | 2.47                     | 0.45              |
| 1:D:142:GLU:O    | 1:D:143:ASP:HB2  | 2.16                     | 0.45              |
| 1:D:391:PRO:HB2  | 1:D:418:LYS:HB2  | 1.98                     | 0.45              |
| 1:D:365:ARG:O    | 1:D:423:GLN:HG2  | 2.16                     | 0.45              |
| 1:F:321:LYS:HB2  | 1:F:322:THR:H    | 1.61                     | 0.45              |
| 1:A:219:LYS:HG3  | 1:A:224:ILE:HG22 | 1.98                     | 0.45              |
| 1:A:235:VAL:HG23 | 1:A:236:VAL:N    | 2.32                     | 0.45              |
| 1:A:553:PRO:HB2  | 1:A:620:VAL:CG2  | 2.33                     | 0.45              |
| 1:A:591:GLU:O    | 1:A:594:VAL:HB   | 2.16                     | 0.45              |
| 1:B:134:CYS:SG   | 1:B:135:GLY:N    | 2.89                     | 0.45              |
| 1:B:268:PRO:C    | 1:B:270:GLU:N    | 2.69                     | 0.45              |
| 1:B:288:GLU:HB3  | 1:B:289:PRO:CD   | 2.33                     | 0.45              |
| 1:B:374:VAL:CG1  | 1:B:744:ARG:HH22 | 2.28                     | 0.45              |
| 1:C:148:ARG:NH2  | 1:C:156:PHE:O    | 2.49                     | 0.45              |
| 1:C:331:ASN:HD22 | 1:C:337:MSE:CA   | 2.20                     | 0.45              |
| 1:D:249:PRO:HG3  | 1:D:300:LEU:CD1  | 2.40                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:286:LYS:HE3  | 1:D:291:PRO:CD   | 2.46                     | 0.45              |
| 1:D:455:LEU:HD13 | 1:D:456:ILE:O    | 2.16                     | 0.45              |
| 1:E:447:ILE:HG22 | 1:E:447:ILE:O    | 2.17                     | 0.45              |
| 1:E:524:VAL:HG23 | 1:E:536:ALA:H    | 1.81                     | 0.45              |
| 1:E:579:PRO:O    | 1:E:582:VAL:HG23 | 2.17                     | 0.45              |
| 1:E:551:TYR:O    | 1:E:628:ARG:HB3  | 2.16                     | 0.45              |
| 1:F:179:THR:HG23 | 1:F:179:THR:O    | 2.17                     | 0.45              |
| 1:F:557:LEU:HD11 | 1:F:621:LEU:HA   | 1.99                     | 0.45              |
| 1:F:585:LEU:HB2  | 1:F:627:ARG:NH1  | 2.31                     | 0.45              |
| 1:A:633:GLU:N    | 1:A:634:PRO:CD   | 2.79                     | 0.45              |
| 1:B:130:VAL:HG11 | 1:B:178:PRO:O    | 2.17                     | 0.45              |
| 1:B:445:ARG:C    | 1:B:447:ILE:H    | 2.20                     | 0.45              |
| 1:B:524:VAL:HG22 | 1:B:536:ALA:H    | 1.81                     | 0.45              |
| 1:A:475:ASN:HD21 | 1:B:590:VAL:N    | 2.14                     | 0.45              |
| 1:B:765:LEU:HD21 | 1:B:770:LEU:CD2  | 2.40                     | 0.45              |
| 1:C:306:MSE:CE   | 1:C:309:TYR:HE2  | 2.30                     | 0.45              |
| 1:C:592:PHE:O    | 1:C:595:VAL:HB   | 2.17                     | 0.45              |
| 1:C:717:TYR:CE1  | 1:C:744:ARG:HG3  | 2.51                     | 0.45              |
| 1:D:202:PRO:O    | 1:D:203:LEU:C    | 2.54                     | 0.45              |
| 1:D:239:LEU:C    | 1:D:239:LEU:HD23 | 2.37                     | 0.45              |
| 1:D:31:ARG:HG2   | 1:D:85:ARG:HA    | 1.98                     | 0.45              |
| 1:D:589:LYS:HG3  | 1:D:590:VAL:HG23 | 1.98                     | 0.45              |
| 1:E:370:VAL:CG2  | 1:E:381:ILE:HD11 | 2.46                     | 0.45              |
| 1:E:397:GLU:HB2  | 1:E:416:ASN:HA   | 1.99                     | 0.45              |
| 1:E:415:LYS:HD3  | 1:E:448:LEU:CD2  | 2.44                     | 0.45              |
| 1:E:414:ALA:HB2  | 1:E:419:VAL:HA   | 1.99                     | 0.45              |
| 1:E:335:MSE:HE1  | 1:E:430:LYS:HG3  | 1.99                     | 0.45              |
| 1:E:450:VAL:HG22 | 1:E:451:LYS:N    | 2.31                     | 0.45              |
| 1:F:252:ILE:HG23 | 1:F:325:TYR:O    | 2.17                     | 0.45              |
| 1:F:270:GLU:N    | 1:F:378:ARG:NH1  | 2.64                     | 0.45              |
| 1:F:398:TYR:CG   | 1:F:398:TYR:O    | 2.70                     | 0.45              |
| 1:F:428:THR:HA   | 1:F:433:VAL:HG11 | 1.99                     | 0.45              |
| 1:F:613:ARG:HA   | 1:F:613:ARG:NE   | 2.29                     | 0.45              |
| 1:F:620:VAL:C    | 1:F:622:LEU:N    | 2.69                     | 0.45              |
| 1:A:124:TYR:CD2  | 1:A:125:MSE:HG2  | 2.51                     | 0.45              |
| 1:A:532:VAL:HG12 | 1:A:533:GLU:N    | 2.32                     | 0.45              |
| 1:A:589:LYS:HG2  | 1:B:475:ASN:OD1  | 2.17                     | 0.45              |
| 1:B:530:GLU:O    | 1:B:531:ASP:HB2  | 2.16                     | 0.45              |
| 1:B:616:ASP:HA   | 1:B:634:PRO:HB2  | 1.99                     | 0.45              |
| 1:B:766:THR:OG1  | 1:B:769:ASP:HB2  | 2.17                     | 0.45              |
| 1:C:279:ARG:CB   | 1:C:309:TYR:HB3  | 2.47                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:394:ILE:CD1  | 1:C:419:VAL:HB   | 2.47                     | 0.45              |
| 1:C:534:ARG:HG2  | 1:C:535:LEU:N    | 2.31                     | 0.45              |
| 1:C:61:TYR:CD2   | 1:C:61:TYR:N     | 2.85                     | 0.45              |
| 1:D:345:PHE:C    | 1:D:347:GLU:H    | 2.20                     | 0.45              |
| 1:D:387:PHE:O    | 1:D:390:LEU:HG   | 2.17                     | 0.45              |
| 1:D:565:TYR:HB3  | 1:D:569:GLU:HB2  | 1.98                     | 0.45              |
| 1:D:582:VAL:C    | 1:D:584:SER:H    | 2.19                     | 0.45              |
| 1:D:581:ALA:HA   | 1:D:584:SER:HB3  | 1.98                     | 0.45              |
| 1:E:151:THR:O    | 1:E:154:LYS:HB2  | 2.16                     | 0.45              |
| 1:E:393:GLU:HA   | 1:E:417:GLY:O    | 2.17                     | 0.45              |
| 1:E:460:LEU:HD12 | 1:E:483:GLN:HB3  | 1.98                     | 0.45              |
| 1:E:629:HIS:HB2  | 1:E:633:GLU:OE1  | 2.17                     | 0.45              |
| 1:F:274:LEU:HB3  | 1:F:307:LEU:HD11 | 1.99                     | 0.45              |
| 1:F:282:ILE:HG23 | 1:F:283:THR:N    | 2.32                     | 0.45              |
| 1:F:369:SER:OG   | 1:F:384:SER:N    | 2.49                     | 0.45              |
| 1:F:429:GLY:HA2  | 1:F:465:ASN:ND2  | 2.32                     | 0.45              |
| 1:A:292:LEU:HB3  | 1:A:296:LEU:HD22 | 1.99                     | 0.45              |
| 1:A:108:ILE:CG1  | 1:A:310:ALA:HA   | 2.34                     | 0.45              |
| 1:A:3:ALA:HB2    | 1:A:47:GLU:CA    | 2.44                     | 0.45              |
| 1:A:653:VAL:CG1  | 1:A:692:ALA:HB3  | 2.46                     | 0.45              |
| 1:B:270:GLU:CD   | 1:B:284:LEU:HD21 | 2.37                     | 0.45              |
| 1:B:250:PHE:CD2  | 1:B:328:THR:HG21 | 2.52                     | 0.45              |
| 1:B:219:LYS:HE2  | 1:B:358:HIS:O    | 2.17                     | 0.45              |
| 1:B:415:LYS:C    | 1:B:417:GLY:H    | 2.19                     | 0.45              |
| 1:B:443:HIS:O    | 1:B:447:ILE:HD12 | 2.16                     | 0.45              |
| 1:C:196:GLN:CG   | 1:C:197:GLU:N    | 2.77                     | 0.45              |
| 1:C:553:PRO:HB2  | 1:C:620:VAL:CG2  | 2.46                     | 0.45              |
| 1:D:306:MSE:HE1  | 1:D:309:TYR:HE2  | 1.82                     | 0.45              |
| 1:D:376:GLY:HA2  | 1:D:726:ARG:HH11 | 1.81                     | 0.45              |
| 1:E:286:LYS:HE3  | 1:E:290:PHE:CB   | 2.46                     | 0.45              |
| 1:E:230:ALA:HB3  | 1:E:324:VAL:CG2  | 2.47                     | 0.45              |
| 1:E:474:ALA:HB2  | 1:E:481:LEU:HD13 | 1.98                     | 0.45              |
| 1:E:521:GLY:CA   | 1:E:610:SER:HA   | 2.46                     | 0.45              |
| 1:F:89:GLU:HG3   | 1:F:175:HIS:CE1  | 2.52                     | 0.45              |
| 1:F:373:PHE:CD2  | 1:F:378:ARG:HD3  | 2.52                     | 0.45              |
| 1:A:207:ALA:HB1  | 1:A:320:SER:CB   | 2.42                     | 0.45              |
| 1:A:263:PHE:HE1  | 1:A:292:LEU:HG   | 1.81                     | 0.45              |
| 1:A:225:HIS:HA   | 1:A:330:ALA:H    | 1.82                     | 0.45              |
| 1:A:428:THR:HG21 | 1:A:466:THR:HG22 | 1.99                     | 0.45              |
| 1:A:466:THR:OG1  | 1:A:467:THR:N    | 2.50                     | 0.45              |
| 1:A:738:VAL:HB   | 1:A:744:ARG:HG2  | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:219:LYS:HB2  | 1:B:357:LEU:HA   | 1.99                     | 0.45              |
| 1:B:371:ILE:CB   | 1:B:380:VAL:HG13 | 2.43                     | 0.45              |
| 1:B:461:HIS:HB2  | 1:B:513:TYR:CB   | 2.47                     | 0.45              |
| 1:B:614:VAL:HG13 | 1:B:666:PHE:CZ   | 2.52                     | 0.45              |
| 1:C:270:GLU:O    | 1:C:274:LEU:HB2  | 2.16                     | 0.45              |
| 1:C:641:PHE:CE2  | 1:C:679:ALA:HA   | 2.52                     | 0.45              |
| 1:D:142:GLU:HB3  | 1:D:150:ASN:C    | 2.36                     | 0.45              |
| 1:D:292:LEU:HD12 | 1:D:296:LEU:HD21 | 1.99                     | 0.45              |
| 1:D:552:TYR:CD1  | 1:D:627:ARG:HG3  | 2.52                     | 0.45              |
| 1:D:739:THR:OG1  | 1:D:740:THR:N    | 2.49                     | 0.45              |
| 1:E:232:ASN:HB3  | 1:E:235:VAL:CG2  | 2.46                     | 0.45              |
| 1:E:504:ILE:CG2  | 1:E:505:GLY:N    | 2.80                     | 0.45              |
| 1:F:11:ILE:HG12  | 1:F:15:VAL:HG21  | 1.98                     | 0.45              |
| 1:F:294:GLU:HG2  | 1:F:294:GLU:O    | 2.17                     | 0.45              |
| 1:F:384:SER:HB2  | 1:F:385:ARG:H    | 1.57                     | 0.45              |
| 1:F:573:VAL:HG13 | 1:F:574:ILE:N    | 2.31                     | 0.45              |
| 1:A:157:PRO:O    | 1:A:184:CYS:HB2  | 2.16                     | 0.44              |
| 1:A:409:ASN:CG   | 1:A:425:ILE:HD11 | 2.37                     | 0.44              |
| 1:A:709:VAL:O    | 1:A:735:ASN:HB2  | 2.17                     | 0.44              |
| 1:B:159:CYS:SG   | 1:B:183:VAL:HG21 | 2.58                     | 0.44              |
| 1:B:270:GLU:OE2  | 1:B:284:LEU:HD21 | 2.17                     | 0.44              |
| 1:B:506:ILE:HG22 | 1:B:508:LEU:HG   | 1.98                     | 0.44              |
| 1:B:568:ASP:O    | 1:B:571:GLU:HB3  | 2.17                     | 0.44              |
| 1:C:144:LEU:HA   | 1:C:145:PRO:C    | 2.37                     | 0.44              |
| 1:C:292:LEU:HD13 | 1:C:293:PRO:CD   | 2.43                     | 0.44              |
| 1:C:487:HIS:CD2  | 1:C:520:TRP:HB3  | 2.51                     | 0.44              |
| 1:D:118:ASP:HA   | 1:D:119:PRO:HD3  | 1.74                     | 0.44              |
| 1:D:191:TYR:HA   | 1:D:195:GLY:O    | 2.17                     | 0.44              |
| 1:D:274:LEU:HD21 | 1:D:282:ILE:HG22 | 1.99                     | 0.44              |
| 1:D:300:LEU:HD21 | 1:D:636:MSE:HE2  | 1.99                     | 0.44              |
| 1:D:447:ILE:HD12 | 1:D:447:ILE:N    | 2.32                     | 0.44              |
| 1:D:246:PRO:HG2  | 1:D:629:HIS:HB3  | 1.97                     | 0.44              |
| 1:E:24:ILE:HG12  | 1:E:56:PHE:CD1   | 2.51                     | 0.44              |
| 1:E:257:ILE:HA   | 1:E:260:VAL:CG2  | 2.46                     | 0.44              |
| 1:E:372:ARG:NH2  | 1:E:717:TYR:HB3  | 2.31                     | 0.44              |
| 1:E:522:GLY:HA2  | 1:E:611:THR:HG23 | 1.98                     | 0.44              |
| 1:E:523:GLU:HB2  | 1:E:525:LEU:HD21 | 1.99                     | 0.44              |
| 1:F:413:VAL:HG11 | 1:F:448:LEU:HD11 | 1.99                     | 0.44              |
| 1:F:44:ILE:HG22  | 1:F:45:VAL:H     | 1.82                     | 0.44              |
| 1:A:116:LEU:HG   | 1:A:117:PHE:N    | 2.32                     | 0.44              |
| 1:A:251:ALA:O    | 1:A:326:VAL:HA   | 2.17                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:399:ASN:HA   | 1:A:414:ALA:O    | 2.17                     | 0.44              |
| 1:A:732:ASN:OD1  | 1:A:733:GLY:N    | 2.51                     | 0.44              |
| 1:B:7:HIS:CD2    | 1:B:43:GLU:HB3   | 2.52                     | 0.44              |
| 1:B:487:HIS:CE1  | 1:B:509:ASP:HB3  | 2.52                     | 0.44              |
| 1:C:66:PRO:HD3   | 1:C:133:ASN:HB3  | 1.99                     | 0.44              |
| 1:C:233:GLU:HB2  | 1:C:293:PRO:HB3  | 1.99                     | 0.44              |
| 1:C:34:VAL:HG23  | 1:C:43:GLU:O     | 2.18                     | 0.44              |
| 1:C:554:LEU:CG   | 1:C:558:MSE:HE3  | 2.47                     | 0.44              |
| 1:C:614:VAL:HG13 | 1:C:666:PHE:CE2  | 2.53                     | 0.44              |
| 1:D:253:MSE:HA   | 1:D:306:MSE:O    | 2.16                     | 0.44              |
| 1:D:312:THR:O    | 1:D:315:ILE:HG22 | 2.18                     | 0.44              |
| 1:D:584:SER:CB   | 1:D:589:LYS:HB3  | 2.47                     | 0.44              |
| 1:D:552:TYR:HD1  | 1:D:627:ARG:HG3  | 1.82                     | 0.44              |
| 1:E:425:ILE:HG22 | 1:E:436:PHE:CD1  | 2.52                     | 0.44              |
| 1:E:543:LEU:HD12 | 1:E:549:ALA:CB   | 2.46                     | 0.44              |
| 1:F:524:VAL:CG2  | 1:F:536:ALA:H    | 2.30                     | 0.44              |
| 1:F:522:GLY:CA   | 1:F:611:THR:HG23 | 2.47                     | 0.44              |
| 1:F:619:ALA:HB2  | 1:F:638:LEU:HD22 | 1.98                     | 0.44              |
| 1:F:62:LYS:C     | 1:F:64:LYS:H     | 2.20                     | 0.44              |
| 1:F:67:LEU:CD1   | 1:F:106:ILE:HD13 | 2.47                     | 0.44              |
| 1:F:639:GLU:OE2  | 1:F:718:ASN:HA   | 2.16                     | 0.44              |
| 1:F:497:GLU:CD   | 1:F:739:THR:HG22 | 2.37                     | 0.44              |
| 1:F:35:LYS:CG    | 1:F:90:LYS:HD2   | 2.41                     | 0.44              |
| 1:A:263:PHE:O    | 1:A:264:ALA:HB2  | 2.18                     | 0.44              |
| 1:A:529:TYR:CE1  | 1:A:759:LEU:HD11 | 2.52                     | 0.44              |
| 1:B:15:VAL:HG21  | 1:B:67:LEU:O     | 2.18                     | 0.44              |
| 1:B:383:ARG:NH1  | 1:B:387:PHE:HB3  | 2.32                     | 0.44              |
| 1:B:401:LEU:HD12 | 1:B:402:ALA:N    | 2.32                     | 0.44              |
| 1:A:772:LEU:HD11 | 1:B:601:LYS:HD3  | 1.99                     | 0.44              |
| 1:C:128:PHE:CD1  | 1:C:186:PRO:HG2  | 2.53                     | 0.44              |
| 1:C:412:GLY:HA3  | 1:C:750:ASN:ND2  | 2.32                     | 0.44              |
| 1:C:501:ASP:O    | 1:C:503:VAL:HG22 | 2.17                     | 0.44              |
| 1:C:567:ILE:HG12 | 1:C:600:ALA:HB1  | 1.99                     | 0.44              |
| 1:D:257:ILE:HD12 | 1:D:260:VAL:CG2  | 2.47                     | 0.44              |
| 1:D:286:LYS:HE3  | 1:D:291:PRO:HD2  | 2.00                     | 0.44              |
| 1:D:281:ILE:CB   | 1:D:370:VAL:HG12 | 2.36                     | 0.44              |
| 1:D:399:ASN:ND2  | 1:D:399:ASN:N    | 2.66                     | 0.44              |
| 1:D:504:ILE:HG13 | 1:D:706:VAL:HG21 | 1.99                     | 0.44              |
| 1:D:601:LYS:HZ2  | 1:E:771:MSE:HE3  | 1.82                     | 0.44              |
| 1:F:329:SER:HA   | 1:F:337:MSE:HE2  | 1.99                     | 0.44              |
| 1:F:567:ILE:HG12 | 1:F:600:ALA:HB1  | 1.98                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:748:GLY:O    | 1:F:751:VAL:HG12 | 2.16                     | 0.44              |
| 1:A:312:THR:HA   | 1:A:315:ILE:HG22 | 2.00                     | 0.44              |
| 1:A:252:ILE:CG2  | 1:A:324:VAL:HB   | 2.48                     | 0.44              |
| 1:B:25:ALA:HA    | 1:B:56:PHE:CE1   | 2.52                     | 0.44              |
| 1:B:319:TRP:O    | 1:B:320:SER:O    | 2.36                     | 0.44              |
| 1:B:337:MSE:CE   | 1:B:367:ASP:HA   | 2.41                     | 0.44              |
| 1:B:6:ILE:HG13   | 1:B:57:ILE:HD12  | 1.98                     | 0.44              |
| 1:C:317:PHE:HE2  | 1:C:323:PRO:CA   | 2.27                     | 0.44              |
| 1:D:219:LYS:HG3  | 1:D:224:ILE:CG2  | 2.43                     | 0.44              |
| 1:D:261:LYS:HD3  | 1:D:266:VAL:CG2  | 2.47                     | 0.44              |
| 1:D:281:ILE:HG23 | 1:D:306:MSE:HG3  | 2.00                     | 0.44              |
| 1:E:286:LYS:CE   | 1:E:290:PHE:HB2  | 2.46                     | 0.44              |
| 1:E:498:LYS:HB2  | 1:E:500:LEU:CD1  | 2.48                     | 0.44              |
| 1:A:35:LYS:HG2   | 1:A:36:ASN:N     | 2.33                     | 0.44              |
| 1:A:401:LEU:HD12 | 1:A:402:ALA:N    | 2.32                     | 0.44              |
| 1:A:582:VAL:HB   | 1:A:583:GLU:OE1  | 2.18                     | 0.44              |
| 1:A:748:GLY:O    | 1:A:751:VAL:HG12 | 2.18                     | 0.44              |
| 1:B:313:HIS:CE1  | 1:B:327:MSE:HE2  | 2.49                     | 0.44              |
| 1:B:422:SER:HA   | 1:B:444:PHE:CZ   | 2.53                     | 0.44              |
| 1:B:495:MSE:HA   | 1:B:500:LEU:HD21 | 2.00                     | 0.44              |
| 1:B:541:TYR:CB   | 1:B:560:ILE:HG22 | 2.48                     | 0.44              |
| 1:B:572:GLY:O    | 1:B:575:ASN:HB2  | 2.17                     | 0.44              |
| 1:B:714:GLY:C    | 1:B:716:ALA:H    | 2.20                     | 0.44              |
| 1:B:738:VAL:HG23 | 1:B:744:ARG:HG2  | 1.99                     | 0.44              |
| 1:C:124:TYR:CE2  | 1:C:125:MSE:HG2  | 2.52                     | 0.44              |
| 1:C:219:LYS:HE3  | 1:C:358:HIS:ND1  | 2.33                     | 0.44              |
| 1:C:30:LEU:O     | 1:C:30:LEU:HD23  | 2.18                     | 0.44              |
| 1:C:278:ARG:CZ   | 1:C:387:PHE:HE1  | 2.29                     | 0.44              |
| 1:C:450:VAL:HG22 | 1:C:451:LYS:N    | 2.30                     | 0.44              |
| 1:C:504:ILE:CG2  | 1:C:505:GLY:N    | 2.81                     | 0.44              |
| 1:C:87:TYR:C     | 1:C:88:ILE:HG13  | 2.37                     | 0.44              |
| 1:D:219:LYS:HA   | 1:D:224:ILE:CG2  | 2.46                     | 0.44              |
| 1:D:286:LYS:NZ   | 1:D:292:LEU:HB2  | 2.32                     | 0.44              |
| 1:D:413:VAL:HG21 | 1:D:448:LEU:HD13 | 1.99                     | 0.44              |
| 1:D:396:PHE:O    | 1:D:417:GLY:HA2  | 2.18                     | 0.44              |
| 1:D:482:LEU:HD11 | 1:D:770:LEU:HD13 | 2.00                     | 0.44              |
| 1:E:410:ALA:CA   | 1:E:425:ILE:HD11 | 2.47                     | 0.44              |
| 1:F:215:ILE:CG2  | 1:F:239:LEU:HD12 | 2.47                     | 0.44              |
| 1:F:230:ALA:HB2  | 1:F:325:TYR:O    | 2.17                     | 0.44              |
| 1:F:219:LYS:HG2  | 1:F:358:HIS:NE2  | 2.32                     | 0.44              |
| 1:F:443:HIS:O    | 1:F:447:ILE:HD12 | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:476:GLU:C    | 1:F:478:ASP:N    | 2.70                     | 0.44              |
| 1:F:736:PHE:CD2  | 1:F:736:PHE:N    | 2.84                     | 0.44              |
| 1:A:144:LEU:HA   | 1:A:145:PRO:C    | 2.37                     | 0.44              |
| 1:A:188:TYR:CE1  | 1:A:358:HIS:HD2  | 2.36                     | 0.44              |
| 1:A:381:ILE:HG13 | 1:A:382:ARG:N    | 2.33                     | 0.44              |
| 1:A:104:PRO:HG3  | 1:A:390:LEU:HD11 | 2.00                     | 0.44              |
| 1:A:415:LYS:O    | 1:A:417:GLY:N    | 2.48                     | 0.44              |
| 1:B:144:LEU:HA   | 1:B:145:PRO:C    | 2.37                     | 0.44              |
| 1:B:370:VAL:HG23 | 1:B:381:ILE:HD11 | 1.99                     | 0.44              |
| 1:A:587:TYR:OH   | 1:B:468:LYS:HG3  | 2.18                     | 0.44              |
| 1:B:653:VAL:CG1  | 1:B:692:ALA:HB3  | 2.43                     | 0.44              |
| 1:C:132:THR:HG23 | 1:C:133:ASN:OD1  | 2.18                     | 0.44              |
| 1:C:134:CYS:SG   | 1:C:135:GLY:N    | 2.90                     | 0.44              |
| 1:C:192:THR:C    | 1:C:194:ASP:N    | 2.69                     | 0.44              |
| 1:C:233:GLU:O    | 1:C:236:VAL:HG12 | 2.18                     | 0.44              |
| 1:C:239:LEU:C    | 1:C:239:LEU:HD23 | 2.38                     | 0.44              |
| 1:C:451:LYS:O    | 1:C:452:ASN:C    | 2.55                     | 0.44              |
| 1:D:130:VAL:HG22 | 1:D:131:CYS:O    | 2.17                     | 0.44              |
| 1:D:312:THR:O    | 1:D:316:LEU:HB2  | 2.18                     | 0.44              |
| 1:D:315:ILE:HG23 | 1:D:316:LEU:N    | 2.32                     | 0.44              |
| 1:D:225:HIS:CA   | 1:D:330:ALA:HB2  | 2.40                     | 0.44              |
| 1:D:216:VAL:HB   | 1:D:354:TYR:HB2  | 1.99                     | 0.44              |
| 1:D:491:ILE:CG2  | 1:D:527:LEU:HD21 | 2.44                     | 0.44              |
| 1:D:599:LEU:O    | 1:D:599:LEU:HD22 | 2.17                     | 0.44              |
| 1:D:541:TYR:CZ   | 1:D:609:SER:HA   | 2.53                     | 0.44              |
| 1:D:759:LEU:CD1  | 1:D:764:TYR:HB2  | 2.46                     | 0.44              |
| 1:E:278:ARG:CZ   | 1:E:387:PHE:HE1  | 2.30                     | 0.44              |
| 1:D:462:PRO:HG2  | 1:E:604:ASN:ND2  | 2.32                     | 0.44              |
| 1:F:142:GLU:HB3  | 1:F:150:ASN:C    | 2.38                     | 0.44              |
| 1:F:286:LYS:HE3  | 1:F:290:PHE:HB2  | 1.99                     | 0.44              |
| 1:F:599:LEU:HD13 | 1:F:599:LEU:O    | 2.17                     | 0.44              |
| 1:F:521:GLY:CA   | 1:F:610:SER:HA   | 2.41                     | 0.44              |
| 1:F:742:VAL:HG13 | 1:F:743:PRO:HD2  | 2.00                     | 0.44              |
| 1:A:612:GLY:HA2  | 1:A:615:LEU:HD23 | 1.99                     | 0.44              |
| 1:A:615:LEU:HD21 | 1:A:635:ALA:CB   | 2.47                     | 0.44              |
| 1:B:210:ILE:HD11 | 1:B:228:CYS:CA   | 2.48                     | 0.44              |
| 1:B:253:MSE:HE2  | 1:B:317:PHE:CD1  | 2.52                     | 0.44              |
| 1:B:405:ALA:H    | 1:B:749:VAL:HG11 | 1.83                     | 0.44              |
| 1:C:283:THR:OG1  | 1:C:372:ARG:HB2  | 2.17                     | 0.44              |
| 1:C:401:LEU:HD12 | 1:C:412:GLY:O    | 2.18                     | 0.44              |
| 1:C:485:GLN:CD   | 1:C:514:GLY:HA2  | 2.37                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:116:LEU:HG   | 1:D:117:PHE:H    | 1.83                     | 0.44              |
| 1:D:269:GLU:HB2  | 1:D:378:ARG:NH2  | 2.33                     | 0.44              |
| 1:D:383:ARG:CZ   | 1:D:421:PRO:HG3  | 2.48                     | 0.44              |
| 1:D:428:THR:HG21 | 1:D:466:THR:HG22 | 2.00                     | 0.44              |
| 1:D:570:LEU:HD12 | 1:D:573:VAL:CG1  | 2.48                     | 0.44              |
| 1:D:727:LYS:O    | 1:D:730:GLU:HG2  | 2.17                     | 0.44              |
| 1:E:677:SER:O    | 1:E:681:ILE:HG12 | 2.17                     | 0.44              |
| 1:F:14:ALA:HA    | 1:F:146:TYR:CD1  | 2.52                     | 0.44              |
| 1:F:1:MSE:HG2    | 1:F:83:PHE:HD1   | 1.83                     | 0.44              |
| 1:F:401:LEU:HD12 | 1:F:412:GLY:O    | 2.18                     | 0.44              |
| 1:F:457:ILE:HA   | 1:F:482:LEU:O    | 2.17                     | 0.44              |
| 1:F:565:TYR:HB3  | 1:F:569:GLU:HG2  | 2.00                     | 0.44              |
| 1:F:9:GLN:HB2    | 1:F:72:ARG:HH21  | 1.83                     | 0.44              |
| 1:A:213:GLY:O    | 1:A:235:VAL:HG11 | 2.17                     | 0.44              |
| 1:A:343:ARG:HG2  | 1:A:343:ARG:HH11 | 1.83                     | 0.44              |
| 1:A:567:ILE:HG23 | 1:A:600:ALA:HB2  | 1.99                     | 0.44              |
| 1:A:584:SER:HA   | 1:A:587:TYR:O    | 2.17                     | 0.44              |
| 1:A:653:VAL:HG23 | 1:A:662:VAL:HA   | 1.99                     | 0.44              |
| 1:B:181:CYS:SG   | 1:B:182:PRO:N    | 2.91                     | 0.44              |
| 1:B:288:GLU:CB   | 1:B:289:PRO:CD   | 2.94                     | 0.44              |
| 1:B:506:ILE:HD11 | 1:B:694:ALA:HA   | 1.99                     | 0.44              |
| 1:B:54:GLU:C     | 1:B:56:PHE:H     | 2.20                     | 0.44              |
| 1:C:18:ARG:O     | 1:C:21:VAL:HG12  | 2.18                     | 0.44              |
| 1:C:45:VAL:HG12  | 1:C:45:VAL:O     | 2.16                     | 0.44              |
| 1:C:485:GLN:HE21 | 1:C:486:HIS:N    | 2.16                     | 0.44              |
| 1:C:560:ILE:HD12 | 1:C:561:LEU:N    | 2.33                     | 0.44              |
| 1:D:252:ILE:HD13 | 1:D:303:ILE:HG22 | 1.99                     | 0.44              |
| 1:D:579:PRO:HB3  | 1:D:626:TYR:CE1  | 2.52                     | 0.44              |
| 1:E:341:ASN:HB3  | 1:E:357:LEU:HD13 | 2.00                     | 0.44              |
| 1:E:756:LEU:HD21 | 1:E:770:LEU:HD22 | 2.00                     | 0.44              |
| 1:F:251:ALA:O    | 1:F:326:VAL:HA   | 2.18                     | 0.44              |
| 1:F:270:GLU:HA   | 1:F:373:PHE:HE2  | 1.83                     | 0.44              |
| 1:F:125:MSE:O    | 1:F:315:ILE:HD12 | 2.18                     | 0.44              |
| 1:F:315:ILE:HG12 | 1:F:319:TRP:CZ3  | 2.53                     | 0.44              |
| 1:F:364:ASN:HD21 | 1:F:443:HIS:CD2  | 2.34                     | 0.44              |
| 1:F:543:LEU:HG   | 1:F:543:LEU:O    | 2.17                     | 0.44              |
| 1:F:707:LYS:HB3  | 1:F:708:ASN:HD22 | 1.83                     | 0.44              |
| 1:A:455:LEU:HB3  | 1:A:480:GLU:HB3  | 2.00                     | 0.44              |
| 1:B:1:MSE:HG2    | 1:B:83:PHE:CD1   | 2.50                     | 0.44              |
| 1:B:293:PRO:O    | 1:B:296:LEU:HD13 | 2.18                     | 0.44              |
| 1:B:249:PRO:CG   | 1:B:300:LEU:HD13 | 2.37                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:412:GLY:HA2  | 1:B:420:TYR:O    | 2.17                     | 0.44              |
| 1:B:413:VAL:CG1  | 1:B:420:TYR:HB2  | 2.47                     | 0.44              |
| 1:B:687:LEU:HD22 | 1:B:724:MSE:SE   | 2.68                     | 0.44              |
| 1:C:261:LYS:HA   | 1:C:261:LYS:HD2  | 1.82                     | 0.44              |
| 1:C:447:ILE:C    | 1:C:448:LEU:HD23 | 2.38                     | 0.44              |
| 1:C:491:ILE:HD12 | 1:C:525:LEU:HD12 | 2.00                     | 0.44              |
| 1:C:518:ASN:HB3  | 1:C:540:TYR:HE2  | 1.82                     | 0.44              |
| 1:C:581:ALA:HA   | 1:C:584:SER:HB3  | 1.98                     | 0.44              |
| 1:C:603:ILE:HD11 | 1:F:772:LEU:HD21 | 1.99                     | 0.44              |
| 1:E:163:ARG:O    | 1:E:166:TYR:HB3  | 2.18                     | 0.44              |
| 1:F:12:VAL:HG22  | 1:F:42:VAL:HG11  | 2.00                     | 0.44              |
| 1:A:163:ARG:HB2  | 1:A:163:ARG:NH1  | 2.21                     | 0.43              |
| 1:A:312:THR:HA   | 1:A:315:ILE:CG2  | 2.48                     | 0.43              |
| 1:A:373:PHE:CE2  | 1:A:378:ARG:HD3  | 2.53                     | 0.43              |
| 1:A:50:GLU:HA    | 1:A:53:ILE:HG22  | 2.01                     | 0.43              |
| 1:A:568:ASP:O    | 1:A:571:GLU:HB3  | 2.16                     | 0.43              |
| 1:B:338:VAL:O    | 1:B:338:VAL:HG13 | 2.18                     | 0.43              |
| 1:B:525:LEU:C    | 1:B:535:LEU:HD13 | 2.39                     | 0.43              |
| 1:B:584:SER:HA   | 1:B:587:TYR:O    | 2.18                     | 0.43              |
| 1:B:651:PHE:CE2  | 1:B:669:ILE:HA   | 2.49                     | 0.43              |
| 1:B:8:VAL:O      | 1:B:9:GLN:HG3    | 2.18                     | 0.43              |
| 1:C:130:VAL:CG2  | 1:C:131:CYS:N    | 2.81                     | 0.43              |
| 1:C:140:ILE:HB   | 1:C:152:THR:HG22 | 1.99                     | 0.43              |
| 1:C:24:ILE:HD11  | 1:C:59:ASP:HB2   | 2.00                     | 0.43              |
| 1:C:299:GLY:C    | 1:C:300:LEU:HG   | 2.38                     | 0.43              |
| 1:C:339:LYS:HB2  | 1:C:339:LYS:HE3  | 1.79                     | 0.43              |
| 1:C:370:VAL:CG2  | 1:C:382:ARG:HB2  | 2.48                     | 0.43              |
| 1:C:409:ASN:CG   | 1:C:410:ALA:H    | 2.22                     | 0.43              |
| 1:D:189:ARG:HD2  | 1:D:191:TYR:OH   | 2.18                     | 0.43              |
| 1:D:383:ARG:NH2  | 1:D:390:LEU:O    | 2.51                     | 0.43              |
| 1:D:504:ILE:CG2  | 1:D:505:GLY:H    | 2.31                     | 0.43              |
| 1:D:643:PHE:C    | 1:D:645:GLY:H    | 2.21                     | 0.43              |
| 1:E:401:LEU:O    | 1:E:456:ILE:HG23 | 2.18                     | 0.43              |
| 1:E:718:ASN:HB3  | 1:E:721:ILE:HB   | 2.00                     | 0.43              |
| 1:F:613:ARG:HH22 | 1:F:628:ARG:HH22 | 1.66                     | 0.43              |
| 1:F:629:HIS:HB2  | 1:F:633:GLU:OE1  | 2.17                     | 0.43              |
| 1:A:148:ARG:HH22 | 1:A:158:MSE:HG3  | 1.83                     | 0.43              |
| 1:A:253:MSE:HE2  | 1:A:317:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:373:PHE:CE1  | 1:A:378:ARG:HB3  | 2.52                     | 0.43              |
| 1:B:65:PRO:HG2   | 1:B:68:ALA:HB3   | 1.99                     | 0.43              |
| 1:B:691:ARG:HH11 | 1:B:695:HIS:HD2  | 1.65                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:492:ALA:CB   | 1:B:756:LEU:HD12 | 2.49                     | 0.43              |
| 1:C:190:LEU:O    | 1:C:196:GLN:HA   | 2.19                     | 0.43              |
| 1:C:226:LEU:HD12 | 1:C:330:ALA:HA   | 2.00                     | 0.43              |
| 1:C:270:GLU:N    | 1:C:378:ARG:HH12 | 2.16                     | 0.43              |
| 1:D:12:VAL:HG22  | 1:D:17:PHE:CE1   | 2.53                     | 0.43              |
| 1:D:198:ILE:HG22 | 1:D:199:TYR:N    | 2.33                     | 0.43              |
| 1:E:181:CYS:SG   | 1:E:182:PRO:CD   | 3.06                     | 0.43              |
| 1:E:334:GLY:HA3  | 1:E:335:MSE:HE2  | 2.00                     | 0.43              |
| 1:D:589:LYS:HG3  | 1:E:475:ASN:HD21 | 1.83                     | 0.43              |
| 1:E:578:CYS:O    | 1:E:578:CYS:SG   | 2.76                     | 0.43              |
| 1:E:616:ASP:HB3  | 1:E:634:PRO:CG   | 2.47                     | 0.43              |
| 1:E:729:VAL:HG12 | 1:E:733:GLY:O    | 2.18                     | 0.43              |
| 1:F:282:ILE:HG22 | 1:F:305:VAL:HB   | 1.99                     | 0.43              |
| 1:F:383:ARG:NH1  | 1:F:387:PHE:HB3  | 2.32                     | 0.43              |
| 1:F:368:ASP:HA   | 1:F:385:ARG:HD3  | 2.00                     | 0.43              |
| 1:F:487:HIS:NE2  | 1:F:520:TRP:HB3  | 2.33                     | 0.43              |
| 1:A:269:GLU:O    | 1:A:272:GLU:HB3  | 2.18                     | 0.43              |
| 1:A:329:SER:HB2  | 1:A:331:ASN:ND2  | 2.31                     | 0.43              |
| 1:A:341:ASN:O    | 1:A:344:ALA:HB3  | 2.18                     | 0.43              |
| 1:A:36:ASN:OD1   | 1:A:42:VAL:HG22  | 2.18                     | 0.43              |
| 1:B:409:ASN:ND2  | 1:B:425:ILE:HD11 | 2.33                     | 0.43              |
| 1:C:18:ARG:NH2   | 1:C:36:ASN:ND2   | 2.66                     | 0.43              |
| 1:C:543:LEU:HD12 | 1:C:549:ALA:HB3  | 2.00                     | 0.43              |
| 1:D:102:ILE:HD12 | 1:D:141:ILE:HG21 | 2.00                     | 0.43              |
| 1:D:204:ARG:C    | 1:D:204:ARG:HD2  | 2.38                     | 0.43              |
| 1:D:338:VAL:HG11 | 1:D:348:LEU:HD11 | 1.99                     | 0.43              |
| 1:D:491:ILE:HD11 | 1:D:505:GLY:C    | 2.38                     | 0.43              |
| 1:E:18:ARG:HD2   | 1:E:175:HIS:ND1  | 2.33                     | 0.43              |
| 1:E:236:VAL:HG13 | 1:E:295:ASN:ND2  | 2.32                     | 0.43              |
| 1:E:620:VAL:HG13 | 1:E:626:TYR:HD1  | 1.82                     | 0.43              |
| 1:F:526:TYR:CB   | 1:F:535:LEU:HD11 | 2.47                     | 0.43              |
| 1:F:52:ASP:O     | 1:F:56:PHE:HB3   | 2.19                     | 0.43              |
| 1:F:757:GLY:C    | 1:F:759:LEU:H    | 2.21                     | 0.43              |
| 1:F:759:LEU:CD1  | 1:F:764:TYR:HB2  | 2.48                     | 0.43              |
| 1:A:406:GLU:HA   | 1:A:466:THR:CG2  | 2.48                     | 0.43              |
| 1:A:560:ILE:HD12 | 1:A:561:LEU:N    | 2.33                     | 0.43              |
| 1:A:603:ILE:HD11 | 1:B:772:LEU:HD21 | 2.00                     | 0.43              |
| 1:A:654:PRO:HG2  | 1:A:661:ARG:HB2  | 2.01                     | 0.43              |
| 1:B:106:ILE:CG2  | 1:B:277:TYR:HB2  | 2.37                     | 0.43              |
| 1:B:396:PHE:CZ   | 1:B:759:LEU:HD13 | 2.54                     | 0.43              |
| 1:B:39:ASP:CG    | 1:B:40:ALA:H     | 2.22                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:209:LEU:O    | 1:C:212:LYS:HB3  | 2.17                     | 0.43              |
| 1:C:348:LEU:HD12 | 1:C:348:LEU:N    | 2.33                     | 0.43              |
| 1:D:163:ARG:HB2  | 1:D:163:ARG:NH1  | 2.28                     | 0.43              |
| 1:D:18:ARG:CB    | 1:D:19:PRO:HD3   | 2.48                     | 0.43              |
| 1:E:395:PRO:HG2  | 1:E:396:PHE:CE2  | 2.52                     | 0.43              |
| 1:F:213:GLY:HA3  | 1:F:235:VAL:HG11 | 2.00                     | 0.43              |
| 1:F:360:ARG:HG2  | 1:F:360:ARG:HH11 | 1.83                     | 0.43              |
| 1:F:564:VAL:HG11 | 1:F:667:GLN:HB2  | 1.99                     | 0.43              |
| 1:F:694:ALA:O    | 1:F:696:THR:N    | 2.51                     | 0.43              |
| 1:F:729:VAL:CB   | 1:F:735:ASN:HD22 | 2.29                     | 0.43              |
| 1:A:151:THR:O    | 1:A:154:LYS:HB2  | 2.18                     | 0.43              |
| 1:A:12:VAL:HG13  | 1:A:17:PHE:CD2   | 2.53                     | 0.43              |
| 1:A:12:VAL:HG13  | 1:A:17:PHE:CG    | 2.53                     | 0.43              |
| 1:A:595:VAL:HG12 | 1:A:595:VAL:O    | 2.18                     | 0.43              |
| 1:B:296:LEU:HD12 | 1:B:296:LEU:N    | 2.32                     | 0.43              |
| 1:B:282:ILE:HA   | 1:B:371:ILE:O    | 2.18                     | 0.43              |
| 1:C:197:GLU:OE2  | 1:D:124:TYR:CD1  | 2.71                     | 0.43              |
| 1:C:364:ASN:HD21 | 1:C:443:HIS:CD2  | 2.35                     | 0.43              |
| 1:C:472:GLU:HG3  | 1:C:473:MSE:N    | 2.32                     | 0.43              |
| 1:C:28:HIS:CE1   | 1:C:55:ALA:HB1   | 2.54                     | 0.43              |
| 1:D:163:ARG:HA   | 1:D:166:TYR:HB3  | 1.99                     | 0.43              |
| 1:D:36:ASN:HA    | 1:D:42:VAL:HG22  | 2.01                     | 0.43              |
| 1:D:595:VAL:HG12 | 1:D:595:VAL:O    | 2.19                     | 0.43              |
| 1:D:20:PHE:CZ    | 1:D:64:LYS:HA    | 2.54                     | 0.43              |
| 1:D:539:ASP:CA   | 1:D:659:LEU:HD11 | 2.45                     | 0.43              |
| 1:E:207:ALA:HB1  | 1:E:320:SER:HB2  | 2.00                     | 0.43              |
| 1:D:589:LYS:CG   | 1:E:475:ASN:HD21 | 2.31                     | 0.43              |
| 1:E:494:VAL:O    | 1:E:496:ALA:N    | 2.51                     | 0.43              |
| 1:F:221:ILE:HG22 | 1:F:360:ARG:HH21 | 1.82                     | 0.43              |
| 1:F:302:THR:O    | 1:F:303:ILE:HG13 | 2.17                     | 0.43              |
| 1:F:323:PRO:HG2  | 1:F:324:VAL:H    | 1.83                     | 0.43              |
| 1:F:227:ALA:HA   | 1:F:326:VAL:O    | 2.19                     | 0.43              |
| 1:A:339:LYS:HG3  | 1:A:365:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:406:GLU:HG3  | 1:A:407:LEU:N    | 2.33                     | 0.43              |
| 1:A:501:ASP:O    | 1:A:502:SER:C    | 2.56                     | 0.43              |
| 1:B:14:ALA:HA    | 1:B:146:TYR:CD1  | 2.54                     | 0.43              |
| 1:B:17:PHE:CZ    | 1:B:60:LEU:HG    | 2.54                     | 0.43              |
| 1:B:230:ALA:HB2  | 1:B:325:TYR:O    | 2.18                     | 0.43              |
| 1:B:323:PRO:HG2  | 1:B:324:VAL:H    | 1.83                     | 0.43              |
| 1:B:219:LYS:CD   | 1:B:358:HIS:H    | 2.30                     | 0.43              |
| 1:C:742:VAL:HG11 | 1:C:751:VAL:HG11 | 2.01                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:102:ILE:CD1  | 1:D:144:LEU:HG   | 2.40                     | 0.43              |
| 1:D:614:VAL:HG13 | 1:D:666:PHE:CZ   | 2.53                     | 0.43              |
| 1:E:279:ARG:CB   | 1:E:309:TYR:HB3  | 2.48                     | 0.43              |
| 1:E:294:GLU:HG2  | 1:E:294:GLU:O    | 2.19                     | 0.43              |
| 1:E:370:VAL:HG22 | 1:E:382:ARG:HB2  | 2.00                     | 0.43              |
| 1:E:425:ILE:HG22 | 1:E:436:PHE:CE1  | 2.53                     | 0.43              |
| 1:E:502:SER:CB   | 1:E:528:GLY:HA2  | 2.48                     | 0.43              |
| 1:E:584:SER:HB3  | 1:E:589:LYS:HB3  | 1.99                     | 0.43              |
| 1:F:383:ARG:CZ   | 1:F:421:PRO:CG   | 2.97                     | 0.43              |
| 1:F:490:HIS:C    | 1:F:492:ALA:N    | 2.70                     | 0.43              |
| 1:F:498:LYS:HB2  | 1:F:500:LEU:CD2  | 2.47                     | 0.43              |
| 1:A:625:ALA:HB2  | 1:A:637:LYS:CD   | 2.42                     | 0.43              |
| 1:A:742:VAL:CG1  | 1:A:751:VAL:HG11 | 2.48                     | 0.43              |
| 1:B:118:ASP:HA   | 1:B:119:PRO:HD3  | 1.74                     | 0.43              |
| 1:B:209:LEU:O    | 1:B:212:LYS:HB2  | 2.18                     | 0.43              |
| 1:B:253:MSE:HE1  | 1:B:313:HIS:ND1  | 2.34                     | 0.43              |
| 1:B:485:GLN:HG3  | 1:B:487:HIS:N    | 2.34                     | 0.43              |
| 1:B:547:ASP:O    | 1:B:550:SER:HB2  | 2.19                     | 0.43              |
| 1:B:593:ASN:C    | 1:B:595:VAL:N    | 2.71                     | 0.43              |
| 1:B:686:HIS:CD2  | 1:B:720:LEU:HD12 | 2.54                     | 0.43              |
| 1:C:261:LYS:CE   | 1:C:266:VAL:HB   | 2.49                     | 0.43              |
| 1:C:224:ILE:CG2  | 1:C:338:VAL:HG13 | 2.48                     | 0.43              |
| 1:C:543:LEU:CD2  | 1:C:543:LEU:H    | 2.23                     | 0.43              |
| 1:C:570:LEU:HA   | 1:C:573:VAL:HG12 | 2.01                     | 0.43              |
| 1:C:5:HIS:HB3    | 1:C:76:LYS:HD2   | 2.00                     | 0.43              |
| 1:D:564:VAL:HG13 | 1:D:667:GLN:NE2  | 2.30                     | 0.43              |
| 1:D:404:GLY:HA2  | 1:D:753:GLN:HE22 | 1.82                     | 0.43              |
| 1:E:19:PRO:HG2   | 1:E:132:THR:HG21 | 2.01                     | 0.43              |
| 1:E:392:ILE:HB   | 1:E:419:VAL:CG1  | 2.49                     | 0.43              |
| 1:F:118:ASP:HA   | 1:F:119:PRO:HD3  | 1.75                     | 0.43              |
| 1:F:263:PHE:O    | 1:F:264:ALA:HB2  | 2.17                     | 0.43              |
| 1:F:485:GLN:HG2  | 1:F:488:TYR:CD2  | 2.54                     | 0.43              |
| 1:F:577:CYS:SG   | 1:F:579:PRO:HD3  | 2.59                     | 0.43              |
| 1:F:739:THR:O    | 1:F:742:VAL:O    | 2.37                     | 0.43              |
| 1:A:110:ASP:O    | 1:A:113:LEU:HB3  | 2.19                     | 0.43              |
| 1:A:226:LEU:HD12 | 1:A:330:ALA:CB   | 2.49                     | 0.43              |
| 1:A:348:LEU:HB3  | 1:A:351:VAL:HB   | 2.01                     | 0.43              |
| 1:A:434:LEU:HD11 | 1:A:465:ASN:O    | 2.18                     | 0.43              |
| 1:A:665:LEU:O    | 1:A:669:ILE:HG13 | 2.18                     | 0.43              |
| 1:A:457:ILE:CG2  | 1:A:753:GLN:HB3  | 2.41                     | 0.43              |
| 1:A:766:THR:OG1  | 1:A:769:ASP:HB2  | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:159:CYS:O    | 1:B:160:ASP:C    | 2.57                     | 0.43              |
| 1:B:286:LYS:CE   | 1:B:290:PHE:HB2  | 2.49                     | 0.43              |
| 1:B:34:VAL:HG12  | 1:B:87:TYR:CE1   | 2.49                     | 0.43              |
| 1:B:406:GLU:HA   | 1:B:466:THR:CG2  | 2.49                     | 0.43              |
| 1:B:494:VAL:HG22 | 1:B:738:VAL:CG2  | 2.40                     | 0.43              |
| 1:B:506:ILE:HD12 | 1:B:725:ILE:HG23 | 2.00                     | 0.43              |
| 1:C:560:ILE:H    | 1:C:560:ILE:HG13 | 1.61                     | 0.43              |
| 1:C:564:VAL:HG11 | 1:C:667:GLN:HG3  | 2.01                     | 0.43              |
| 1:C:621:LEU:O    | 1:C:622:LEU:HD23 | 2.18                     | 0.43              |
| 1:C:396:PHE:CZ   | 1:C:759:LEU:HD13 | 2.54                     | 0.43              |
| 1:D:319:TRP:O    | 1:D:320:SER:C    | 2.55                     | 0.43              |
| 1:D:415:LYS:C    | 1:D:417:GLY:H    | 2.22                     | 0.43              |
| 1:D:738:VAL:HG11 | 1:D:742:VAL:HG12 | 2.01                     | 0.43              |
| 1:D:380:VAL:CG2  | 1:D:740:THR:HG23 | 2.47                     | 0.43              |
| 1:E:171:ASN:HD21 | 1:E:173:ARG:HB2  | 1.82                     | 0.43              |
| 1:E:286:LYS:HE3  | 1:E:290:PHE:CA   | 2.48                     | 0.43              |
| 1:E:286:LYS:HE3  | 1:E:290:PHE:HA   | 2.01                     | 0.43              |
| 1:E:370:VAL:H    | 1:E:382:ARG:CB   | 2.32                     | 0.43              |
| 1:F:123:ARG:NH2  | 1:F:173:ARG:HG2  | 2.33                     | 0.43              |
| 1:F:12:VAL:HG23  | 1:F:17:PHE:CG    | 2.53                     | 0.43              |
| 1:F:25:ALA:HB1   | 1:F:30:LEU:O     | 2.19                     | 0.43              |
| 1:A:584:SER:CB   | 1:A:589:LYS:HB3  | 2.43                     | 0.43              |
| 1:A:654:PRO:O    | 1:A:660:ILE:HG23 | 2.19                     | 0.43              |
| 1:B:110:ASP:O    | 1:B:113:LEU:HB3  | 2.19                     | 0.43              |
| 1:A:468:LYS:HA   | 1:B:587:TYR:OH   | 2.18                     | 0.43              |
| 1:B:743:PRO:HG2  | 1:B:748:GLY:HA3  | 2.00                     | 0.43              |
| 1:C:372:ARG:HD2  | 1:C:373:PHE:N    | 2.34                     | 0.43              |
| 1:D:252:ILE:CG2  | 1:D:324:VAL:HB   | 2.49                     | 0.43              |
| 1:D:455:LEU:HD12 | 1:D:455:LEU:C    | 2.39                     | 0.43              |
| 1:D:583:GLU:HG3  | 1:D:592:PHE:CD1  | 2.53                     | 0.43              |
| 1:E:154:LYS:O    | 1:E:154:LYS:HD3  | 2.19                     | 0.43              |
| 1:E:170:LEU:HD12 | 1:E:170:LEU:N    | 2.34                     | 0.43              |
| 1:E:315:ILE:CG2  | 1:E:316:LEU:N    | 2.82                     | 0.43              |
| 1:F:371:ILE:HD12 | 1:F:380:VAL:CG2  | 2.44                     | 0.43              |
| 1:F:456:ILE:CG2  | 1:F:457:ILE:N    | 2.81                     | 0.43              |
| 1:A:177:GLU:HB2  | 1:A:178:PRO:CD   | 2.49                     | 0.43              |
| 1:A:29:ASN:O     | 1:A:31:ARG:HD2   | 2.19                     | 0.43              |
| 1:A:339:LYS:HE2  | 1:A:365:ARG:HH12 | 1.84                     | 0.43              |
| 1:A:34:VAL:O     | 1:A:34:VAL:HG13  | 2.19                     | 0.43              |
| 1:A:476:GLU:C    | 1:A:478:ASP:N    | 2.72                     | 0.43              |
| 1:B:545:GLY:HA3  | 1:B:548:LEU:HD12 | 2.01                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:614:VAL:HG12 | 1:B:618:ILE:HD11 | 2.01                     | 0.43              |
| 1:C:399:ASN:N    | 1:C:399:ASN:ND2  | 2.67                     | 0.43              |
| 1:C:768:GLU:C    | 1:C:770:LEU:H    | 2.23                     | 0.43              |
| 1:D:108:ILE:HG13 | 1:D:310:ALA:HA   | 2.01                     | 0.43              |
| 1:D:488:TYR:HE1  | 1:D:525:LEU:HB3  | 1.84                     | 0.43              |
| 1:D:487:HIS:HE1  | 1:D:509:ASP:HB3  | 1.81                     | 0.43              |
| 1:E:283:THR:OG1  | 1:E:372:ARG:HB2  | 2.19                     | 0.43              |
| 1:E:757:GLY:C    | 1:E:759:LEU:N    | 2.73                     | 0.43              |
| 1:F:578:CYS:O    | 1:F:578:CYS:SG   | 2.77                     | 0.43              |
| 1:F:24:ILE:HD13  | 1:F:60:LEU:HD13  | 2.00                     | 0.43              |
| 1:B:116:LEU:HD23 | 1:B:129:ILE:HG21 | 2.01                     | 0.42              |
| 1:B:131:CYS:SG   | 1:B:133:ASN:HB2  | 2.59                     | 0.42              |
| 1:C:183:VAL:CG2  | 1:C:184:CYS:N    | 2.81                     | 0.42              |
| 1:C:204:ARG:O    | 1:C:204:ARG:HD2  | 2.18                     | 0.42              |
| 1:C:263:PHE:O    | 1:C:264:ALA:HB2  | 2.18                     | 0.42              |
| 1:C:138:PHE:CB   | 1:C:389:PRO:HD3  | 2.47                     | 0.42              |
| 1:C:591:GLU:O    | 1:C:595:VAL:HG23 | 2.19                     | 0.42              |
| 1:C:74:GLU:HG2   | 1:C:74:GLU:O     | 2.18                     | 0.42              |
| 1:D:520:TRP:HZ2  | 1:D:534:ARG:HH21 | 1.67                     | 0.42              |
| 1:D:711:LEU:O    | 1:D:712:SER:HB2  | 2.19                     | 0.42              |
| 1:E:225:HIS:HB2  | 1:E:328:THR:O    | 2.19                     | 0.42              |
| 1:E:450:VAL:HG22 | 1:E:451:LYS:H    | 1.84                     | 0.42              |
| 1:E:455:LEU:HA   | 1:E:479:VAL:CG1  | 2.49                     | 0.42              |
| 1:E:755:PHE:CG   | 1:E:755:PHE:O    | 2.72                     | 0.42              |
| 1:F:265:TYR:HD2  | 1:F:265:TYR:N    | 2.14                     | 0.42              |
| 1:F:524:VAL:O    | 1:F:525:LEU:HD23 | 2.19                     | 0.42              |
| 1:F:381:ILE:HG22 | 1:F:717:TYR:CZ   | 2.54                     | 0.42              |
| 1:A:265:TYR:O    | 1:A:284:LEU:HB2  | 2.18                     | 0.42              |
| 1:A:399:ASN:O    | 1:A:454:ASP:HB2  | 2.19                     | 0.42              |
| 1:A:726:ARG:HH21 | 1:A:727:LYS:CG   | 2.32                     | 0.42              |
| 1:B:171:ASN:ND2  | 1:B:173:ARG:H    | 2.17                     | 0.42              |
| 1:B:427:ASN:HD21 | 1:B:429:GLY:H    | 1.65                     | 0.42              |
| 1:B:540:TYR:CD1  | 1:B:540:TYR:N    | 2.87                     | 0.42              |
| 1:B:654:PRO:HG2  | 1:B:661:ARG:HB2  | 2.01                     | 0.42              |
| 1:B:670:LEU:O    | 1:B:673:ILE:HG12 | 2.19                     | 0.42              |
| 1:B:57:ILE:HG21  | 1:B:75:LYS:HE2   | 2.01                     | 0.42              |
| 1:C:129:ILE:HG13 | 1:C:130:VAL:H    | 1.84                     | 0.42              |
| 1:C:503:VAL:HA   | 1:C:706:VAL:CG1  | 2.50                     | 0.42              |
| 1:D:21:VAL:HA    | 1:D:24:ILE:CG2   | 2.49                     | 0.42              |
| 1:D:335:MSE:HE2  | 1:D:335:MSE:N    | 2.33                     | 0.42              |
| 1:D:719:GLU:O    | 1:D:719:GLU:HG3  | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:210:ILE:HD11 | 1:E:228:CYS:N    | 2.34                     | 0.42              |
| 1:E:225:HIS:HE2  | 1:E:327:MSE:HE3  | 1.84                     | 0.42              |
| 1:E:371:ILE:CB   | 1:E:380:VAL:HG13 | 2.41                     | 0.42              |
| 1:E:381:ILE:HG22 | 1:E:717:TYR:CE1  | 2.54                     | 0.42              |
| 1:D:475:ASN:HD22 | 1:E:591:GLU:HG2  | 1.83                     | 0.42              |
| 1:F:371:ILE:CG1  | 1:F:380:VAL:HG22 | 2.49                     | 0.42              |
| 1:F:541:TYR:OH   | 1:F:610:SER:N    | 2.52                     | 0.42              |
| 1:A:181:CYS:SG   | 1:A:182:PRO:N    | 2.91                     | 0.42              |
| 1:A:370:VAL:CG2  | 1:A:382:ARG:HB2  | 2.50                     | 0.42              |
| 1:A:485:GLN:HB3  | 1:A:488:TYR:HD2  | 1.83                     | 0.42              |
| 1:A:567:ILE:HG12 | 1:A:600:ALA:HB1  | 2.00                     | 0.42              |
| 1:B:552:TYR:HA   | 1:B:553:PRO:HD2  | 1.92                     | 0.42              |
| 1:B:381:ILE:HG22 | 1:B:717:TYR:CE1  | 2.54                     | 0.42              |
| 1:B:9:GLN:HG2    | 1:B:40:ALA:HA    | 2.00                     | 0.42              |
| 1:C:188:TYR:CE1  | 1:C:312:THR:HG21 | 2.54                     | 0.42              |
| 1:C:372:ARG:O    | 1:C:379:ALA:O    | 2.37                     | 0.42              |
| 1:C:364:ASN:ND2  | 1:C:443:HIS:NE2  | 2.68                     | 0.42              |
| 1:C:628:ARG:CZ   | 1:C:632:GLY:H    | 2.32                     | 0.42              |
| 1:D:543:LEU:CD2  | 1:D:543:LEU:N    | 2.82                     | 0.42              |
| 1:E:523:GLU:CD   | 1:E:537:HIS:HB2  | 2.40                     | 0.42              |
| 1:D:475:ASN:ND2  | 1:E:591:GLU:HG2  | 2.34                     | 0.42              |
| 1:F:38:GLY:CA    | 1:F:144:LEU:HB3  | 2.49                     | 0.42              |
| 1:F:210:ILE:HD11 | 1:F:228:CYS:N    | 2.33                     | 0.42              |
| 1:F:219:LYS:HA   | 1:F:224:ILE:HG23 | 2.00                     | 0.42              |
| 1:F:537:HIS:HE2  | 1:F:659:LEU:HD22 | 1.82                     | 0.42              |
| 1:A:172:ARG:C    | 1:A:174:TYR:H    | 2.23                     | 0.42              |
| 1:A:504:ILE:HG22 | 1:A:709:VAL:HG12 | 2.00                     | 0.42              |
| 1:A:702:ARG:C    | 1:A:704:PHE:H    | 2.22                     | 0.42              |
| 1:B:18:ARG:HB3   | 1:B:175:HIS:ND1  | 2.34                     | 0.42              |
| 1:B:256:ASP:O    | 1:B:258:GLU:N    | 2.52                     | 0.42              |
| 1:B:391:PRO:HB2  | 1:B:418:LYS:HB2  | 2.01                     | 0.42              |
| 1:B:455:LEU:HD13 | 1:B:456:ILE:O    | 2.20                     | 0.42              |
| 1:C:204:ARG:HA   | 1:C:319:TRP:CZ3  | 2.54                     | 0.42              |
| 1:C:35:LYS:O     | 1:C:36:ASN:HB2   | 2.20                     | 0.42              |
| 1:C:639:GLU:OE2  | 1:C:718:ASN:HA   | 2.19                     | 0.42              |
| 1:D:171:ASN:HD22 | 1:D:173:ARG:H    | 1.67                     | 0.42              |
| 1:D:486:HIS:CD2  | 1:D:490:HIS:HE2  | 2.36                     | 0.42              |
| 1:D:30:LEU:HD22  | 1:D:52:ASP:O     | 2.19                     | 0.42              |
| 1:D:738:VAL:HG12 | 1:D:742:VAL:O    | 2.19                     | 0.42              |
| 1:E:107:ALA:HB2  | 1:E:309:TYR:HB2  | 2.01                     | 0.42              |
| 1:E:261:LYS:NZ   | 1:E:266:VAL:HB   | 2.34                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:30:LEU:HD23  | 1:E:30:LEU:O     | 2.19                     | 0.42              |
| 1:E:138:PHE:HB2  | 1:E:389:PRO:HD3  | 2.01                     | 0.42              |
| 1:E:405:ALA:O    | 1:E:466:THR:HG21 | 2.19                     | 0.42              |
| 1:E:528:GLY:O    | 1:E:529:TYR:C    | 2.56                     | 0.42              |
| 1:E:570:LEU:HA   | 1:E:573:VAL:HG12 | 2.01                     | 0.42              |
| 1:E:771:MSE:O    | 1:E:772:LEU:HD23 | 2.19                     | 0.42              |
| 1:F:369:SER:HB2  | 1:F:385:ARG:HB2  | 2.00                     | 0.42              |
| 1:F:504:ILE:CG2  | 1:F:505:GLY:H    | 2.33                     | 0.42              |
| 1:A:215:ILE:HD11 | 1:A:352:ALA:HA   | 2.02                     | 0.42              |
| 1:A:210:ILE:HD11 | 1:A:228:CYS:HA   | 2.02                     | 0.42              |
| 1:A:253:MSE:SE   | 1:A:313:HIS:ND1  | 3.03                     | 0.42              |
| 1:A:587:TYR:OH   | 1:B:468:LYS:HA   | 2.19                     | 0.42              |
| 1:A:687:LEU:HD22 | 1:A:724:MSE:CE   | 2.44                     | 0.42              |
| 1:A:708:ASN:N    | 1:A:708:ASN:OD1  | 2.52                     | 0.42              |
| 1:B:251:ALA:HB3  | 1:B:327:MSE:O    | 2.20                     | 0.42              |
| 1:B:385:ARG:HG3  | 1:B:386:GLY:N    | 2.35                     | 0.42              |
| 1:B:528:GLY:H    | 1:B:532:VAL:HG22 | 1.85                     | 0.42              |
| 1:C:18:ARG:HH21  | 1:C:36:ASN:ND2   | 2.15                     | 0.42              |
| 1:C:204:ARG:HG2  | 1:C:319:TRP:CH2  | 2.55                     | 0.42              |
| 1:C:232:ASN:CG   | 1:C:235:VAL:HG22 | 2.40                     | 0.42              |
| 1:C:260:VAL:HG12 | 1:C:266:VAL:CG2  | 2.49                     | 0.42              |
| 1:C:487:HIS:HE1  | 1:C:509:ASP:HB3  | 1.85                     | 0.42              |
| 1:C:526:TYR:CB   | 1:C:535:LEU:HD11 | 2.49                     | 0.42              |
| 1:D:401:LEU:O    | 1:D:456:ILE:HA   | 2.20                     | 0.42              |
| 1:D:610:SER:HB3  | 1:D:613:ARG:CG   | 2.50                     | 0.42              |
| 1:E:137:ARG:C    | 1:E:141:ILE:HG13 | 2.39                     | 0.42              |
| 1:E:199:TYR:CG   | 1:E:200:GLY:N    | 2.87                     | 0.42              |
| 1:E:451:LYS:O    | 1:E:452:ASN:C    | 2.57                     | 0.42              |
| 1:E:599:LEU:O    | 1:E:599:LEU:HD22 | 2.19                     | 0.42              |
| 1:F:23:ARG:HD3   | 1:F:169:PRO:O    | 2.19                     | 0.42              |
| 1:F:399:ASN:O    | 1:F:454:ASP:HB2  | 2.20                     | 0.42              |
| 1:F:20:PHE:CE1   | 1:F:60:LEU:HD12  | 2.54                     | 0.42              |
| 1:A:427:ASN:C    | 1:A:429:GLY:H    | 2.22                     | 0.42              |
| 1:A:438:ARG:HG2  | 1:A:438:ARG:NH1  | 2.34                     | 0.42              |
| 1:A:504:ILE:CG2  | 1:A:505:GLY:N    | 2.82                     | 0.42              |
| 1:B:19:PRO:HA    | 1:B:174:TYR:CD1  | 2.54                     | 0.42              |
| 1:B:406:GLU:HG3  | 1:B:407:LEU:N    | 2.35                     | 0.42              |
| 1:B:413:VAL:O    | 1:B:420:TYR:N    | 2.53                     | 0.42              |
| 1:B:570:LEU:HD12 | 1:B:573:VAL:CG1  | 2.50                     | 0.42              |
| 1:B:639:GLU:HB2  | 1:B:718:ASN:HD21 | 1.83                     | 0.42              |
| 1:C:270:GLU:HA   | 1:C:373:PHE:HE2  | 1.84                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:383:ARG:CZ   | 1:C:387:PHE:HB3  | 2.50                     | 0.42              |
| 1:C:9:GLN:HE21   | 1:C:41:GLY:N     | 2.16                     | 0.42              |
| 1:C:508:LEU:CD2  | 1:C:611:THR:HG21 | 2.48                     | 0.42              |
| 1:C:88:ILE:CG2   | 1:C:89:GLU:H     | 2.23                     | 0.42              |
| 1:D:664:GLU:HA   | 1:D:667:GLN:HG3  | 2.01                     | 0.42              |
| 1:E:438:ARG:NH2  | 1:E:469:LEU:HD21 | 2.34                     | 0.42              |
| 1:E:503:VAL:HA   | 1:E:706:VAL:HG11 | 2.00                     | 0.42              |
| 1:E:58:GLU:HA    | 1:E:61:TYR:HD2   | 1.85                     | 0.42              |
| 1:E:729:VAL:CB   | 1:E:735:ASN:HD22 | 2.30                     | 0.42              |
| 1:F:177:GLU:N    | 1:F:178:PRO:HD2  | 2.35                     | 0.42              |
| 1:F:19:PRO:HA    | 1:F:174:TYR:HD1  | 1.81                     | 0.42              |
| 1:F:301:HIS:CD2  | 1:F:302:THR:N    | 2.87                     | 0.42              |
| 1:F:343:ARG:HD3  | 1:F:343:ARG:HA   | 1.81                     | 0.42              |
| 1:F:500:LEU:HD22 | 1:F:736:PHE:CZ   | 2.54                     | 0.42              |
| 1:F:520:TRP:HZ2  | 1:F:534:ARG:HH21 | 1.67                     | 0.42              |
| 1:A:229:ASP:OD1  | 1:A:322:THR:HG21 | 2.20                     | 0.42              |
| 1:A:365:ARG:HH21 | 1:A:436:PHE:HD2  | 1.67                     | 0.42              |
| 1:A:495:MSE:HE2  | 1:A:755:PHE:HZ   | 1.84                     | 0.42              |
| 1:A:765:LEU:HD12 | 1:A:766:THR:H    | 1.84                     | 0.42              |
| 1:A:88:ILE:HD12  | 1:A:88:ILE:N     | 2.34                     | 0.42              |
| 1:B:102:ILE:CD1  | 1:B:103:PRO:HD2  | 2.50                     | 0.42              |
| 1:C:122:LYS:HD3  | 1:D:198:ILE:HD11 | 2.01                     | 0.42              |
| 1:C:148:ARG:HH21 | 1:C:158:MSE:N    | 2.18                     | 0.42              |
| 1:C:482:LEU:HD21 | 1:C:757:GLY:HA2  | 2.01                     | 0.42              |
| 1:C:20:PHE:CE1   | 1:C:60:LEU:HD12  | 2.55                     | 0.42              |
| 1:C:649:LEU:CG   | 1:C:650:LYS:H    | 2.33                     | 0.42              |
| 1:C:381:ILE:HG22 | 1:C:717:TYR:CZ   | 2.55                     | 0.42              |
| 1:C:718:ASN:HD22 | 1:C:720:LEU:HB2  | 1.83                     | 0.42              |
| 1:D:252:ILE:HG12 | 1:D:296:LEU:HD23 | 2.01                     | 0.42              |
| 1:D:253:MSE:O    | 1:D:317:PHE:HZ   | 2.01                     | 0.42              |
| 1:D:320:SER:HB3  | 1:D:325:TYR:OH   | 2.19                     | 0.42              |
| 1:D:383:ARG:HD2  | 1:D:387:PHE:HD2  | 1.84                     | 0.42              |
| 1:D:7:HIS:NE2    | 1:D:43:GLU:HG3   | 2.35                     | 0.42              |
| 1:D:520:TRP:HE1  | 1:D:534:ARG:NH2  | 2.17                     | 0.42              |
| 1:D:597:ASN:HB3  | 1:D:601:LYS:HE3  | 2.01                     | 0.42              |
| 1:D:726:ARG:HH21 | 1:D:727:LYS:HG2  | 1.85                     | 0.42              |
| 1:E:293:PRO:C    | 1:E:295:ASN:N    | 2.72                     | 0.42              |
| 1:E:503:VAL:HG11 | 1:E:708:ASN:OD1  | 2.19                     | 0.42              |
| 1:F:171:ASN:HD21 | 1:F:173:ARG:HB2  | 1.82                     | 0.42              |
| 1:F:216:VAL:HG23 | 1:F:354:TYR:C    | 2.40                     | 0.42              |
| 1:F:766:THR:HG21 | 1:F:769:ASP:OD2  | 2.19                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:487:HIS:NE2  | 1:A:521:GLY:HA2  | 2.35                     | 0.42              |
| 1:A:561:LEU:CB   | 1:A:570:LEU:HD13 | 2.50                     | 0.42              |
| 1:A:577:CYS:SG   | 1:A:579:PRO:HD3  | 2.59                     | 0.42              |
| 1:B:264:ALA:CB   | 1:B:286:LYS:HA   | 2.50                     | 0.42              |
| 1:B:226:LEU:CD1  | 1:B:330:ALA:HA   | 2.50                     | 0.42              |
| 1:B:420:TYR:HB3  | 1:B:444:PHE:HE1  | 1.85                     | 0.42              |
| 1:B:544:PRO:O    | 1:B:549:ALA:HB2  | 2.20                     | 0.42              |
| 1:B:580:LYS:C    | 1:B:582:VAL:H    | 2.22                     | 0.42              |
| 1:B:751:VAL:CG1  | 1:B:752:GLY:N    | 2.82                     | 0.42              |
| 1:C:253:MSE:HB3  | 1:C:325:TYR:HB2  | 2.02                     | 0.42              |
| 1:C:102:ILE:HG21 | 1:C:389:PRO:HG3  | 2.01                     | 0.42              |
| 1:C:487:HIS:CE1  | 1:C:509:ASP:HB3  | 2.55                     | 0.42              |
| 1:D:65:PRO:HB2   | 1:D:66:PRO:HD2   | 2.00                     | 0.42              |
| 1:E:247:GLN:HG3  | 1:E:298:PRO:HG2  | 2.02                     | 0.42              |
| 1:E:34:VAL:HG23  | 1:E:44:ILE:HG12  | 2.02                     | 0.42              |
| 1:E:530:GLU:HG3  | 1:E:531:ASP:OD2  | 2.20                     | 0.42              |
| 1:E:543:LEU:HB2  | 1:E:549:ALA:CB   | 2.50                     | 0.42              |
| 1:E:8:VAL:HG13   | 1:E:70:ILE:HG23  | 2.01                     | 0.42              |
| 1:E:79:PRO:HA    | 1:E:80:PRO:HD3   | 1.89                     | 0.42              |
| 1:F:293:PRO:C    | 1:F:295:ASN:H    | 2.23                     | 0.42              |
| 1:F:35:LYS:HE2   | 1:F:90:LYS:HZ3   | 1.82                     | 0.42              |
| 1:F:412:GLY:HA2  | 1:F:420:TYR:O    | 2.18                     | 0.42              |
| 1:F:621:LEU:HD22 | 1:F:666:PHE:HD1  | 1.84                     | 0.42              |
| 1:F:702:ARG:NH2  | 1:F:731:ALA:O    | 2.53                     | 0.42              |
| 1:A:123:ARG:NH2  | 1:A:173:ARG:NE   | 2.68                     | 0.42              |
| 1:A:235:VAL:O    | 1:A:238:GLU:HB2  | 2.19                     | 0.42              |
| 1:B:257:ILE:O    | 1:B:260:VAL:HB   | 2.20                     | 0.42              |
| 1:B:610:SER:HB3  | 1:B:613:ARG:CG   | 2.50                     | 0.42              |
| 1:B:672:ALA:O    | 1:B:676:ALA:HB3  | 2.20                     | 0.42              |
| 1:B:738:VAL:HG11 | 1:B:742:VAL:HG12 | 2.01                     | 0.42              |
| 1:C:202:PRO:O    | 1:C:203:LEU:C    | 2.57                     | 0.42              |
| 1:C:385:ARG:CG   | 1:C:386:GLY:N    | 2.74                     | 0.42              |
| 1:C:424:TYR:C    | 1:C:426:GLY:H    | 2.23                     | 0.42              |
| 1:D:284:LEU:O    | 1:D:302:THR:HA   | 2.19                     | 0.42              |
| 1:D:287:LYS:HG3  | 1:D:288:GLU:N    | 2.35                     | 0.42              |
| 1:E:11:ILE:HG23  | 1:E:12:VAL:N     | 2.34                     | 0.42              |
| 1:E:19:PRO:HA    | 1:E:174:TYR:CD1  | 2.54                     | 0.42              |
| 1:E:702:ARG:C    | 1:E:704:PHE:H    | 2.23                     | 0.42              |
| 1:F:38:GLY:HA2   | 1:F:145:PRO:HA   | 2.01                     | 0.42              |
| 1:F:215:ILE:O    | 1:F:215:ILE:HG13 | 2.20                     | 0.42              |
| 1:F:279:ARG:HG3  | 1:F:309:TYR:CB   | 2.50                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:385:ARG:HA   | 1:F:385:ARG:HD2  | 1.91                     | 0.42              |
| 1:A:197:GLU:C    | 1:A:198:ILE:HG12 | 2.41                     | 0.42              |
| 1:A:230:ALA:O    | 1:A:292:LEU:HD12 | 2.20                     | 0.42              |
| 1:A:247:GLN:NE2  | 1:A:298:PRO:HG2  | 2.34                     | 0.42              |
| 1:A:670:LEU:O    | 1:A:673:ILE:HG12 | 2.20                     | 0.42              |
| 1:B:16:GLY:HA3   | 1:B:132:THR:HG23 | 2.02                     | 0.42              |
| 1:B:225:HIS:CD2  | 1:B:225:HIS:N    | 2.86                     | 0.42              |
| 1:B:281:ILE:HA   | 1:B:305:VAL:O    | 2.19                     | 0.42              |
| 1:B:524:VAL:O    | 1:B:535:LEU:HB2  | 2.20                     | 0.42              |
| 1:C:466:THR:OG1  | 1:C:467:THR:N    | 2.53                     | 0.42              |
| 1:C:515:THR:O    | 1:C:516:ASP:HB2  | 2.18                     | 0.42              |
| 1:C:301:HIS:ND1  | 1:C:640:SER:HB3  | 2.35                     | 0.42              |
| 1:C:65:PRO:HG2   | 1:C:68:ALA:HB3   | 2.00                     | 0.42              |
| 1:C:766:THR:OG1  | 1:C:769:ASP:HB2  | 2.20                     | 0.42              |
| 1:D:239:LEU:HD22 | 1:D:250:PHE:CZ   | 2.55                     | 0.42              |
| 1:D:329:SER:HB2  | 1:D:331:ASN:ND2  | 2.29                     | 0.42              |
| 1:D:329:SER:CA   | 1:D:337:MSE:HE2  | 2.49                     | 0.42              |
| 1:D:580:LYS:HD2  | 1:D:590:VAL:HA   | 2.01                     | 0.42              |
| 1:D:690:ALA:HB2  | 1:D:721:ILE:HG23 | 2.02                     | 0.42              |
| 1:E:12:VAL:O     | 1:E:12:VAL:HG22  | 2.20                     | 0.42              |
| 1:E:183:VAL:CG2  | 1:E:184:CYS:H    | 2.31                     | 0.42              |
| 1:E:748:GLY:O    | 1:E:751:VAL:HG12 | 2.19                     | 0.42              |
| 1:F:210:ILE:HD11 | 1:F:227:ALA:O    | 2.20                     | 0.42              |
| 1:F:339:LYS:HG3  | 1:F:365:ARG:NH1  | 2.34                     | 0.42              |
| 1:F:376:GLY:HA2  | 1:F:726:ARG:HH11 | 1.84                     | 0.42              |
| 1:F:391:PRO:C    | 1:F:392:ILE:HD12 | 2.41                     | 0.42              |
| 1:F:481:LEU:HD12 | 1:F:482:LEU:H    | 1.84                     | 0.42              |
| 1:F:536:ALA:HA   | 1:F:658:GLU:O    | 2.20                     | 0.42              |
| 1:A:123:ARG:HE   | 1:A:173:ARG:NH2  | 2.16                     | 0.41              |
| 1:A:209:LEU:N    | 1:A:209:LEU:HD12 | 2.35                     | 0.41              |
| 1:A:359:ASN:O    | 1:A:360:ARG:C    | 2.58                     | 0.41              |
| 1:A:589:LYS:CG   | 1:A:590:VAL:H    | 2.22                     | 0.41              |
| 1:B:166:TYR:CZ   | 1:B:175:HIS:HA   | 2.55                     | 0.41              |
| 1:B:15:VAL:HG13  | 1:B:67:LEU:HB2   | 2.01                     | 0.41              |
| 1:C:209:LEU:HD12 | 1:C:209:LEU:N    | 2.35                     | 0.41              |
| 1:D:278:ARG:CG   | 1:D:280:PRO:HD3  | 2.49                     | 0.41              |
| 1:D:561:LEU:HB2  | 1:D:570:LEU:CD1  | 2.50                     | 0.41              |
| 1:D:639:GLU:HB2  | 1:D:718:ASN:HD21 | 1.85                     | 0.41              |
| 1:E:543:LEU:HD23 | 1:E:606:ALA:O    | 2.20                     | 0.41              |
| 1:F:383:ARG:CZ   | 1:F:387:PHE:HB3  | 2.50                     | 0.41              |
| 1:F:615:LEU:HD23 | 1:F:635:ALA:HB1  | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:502:SER:HB3  | 1:A:527:LEU:O    | 2.20                     | 0.41              |
| 1:B:67:LEU:HD22  | 1:B:106:ILE:HD13 | 2.01                     | 0.41              |
| 1:B:166:TYR:CE1  | 1:B:175:HIS:HA   | 2.54                     | 0.41              |
| 1:B:281:ILE:CB   | 1:B:370:VAL:HG12 | 2.42                     | 0.41              |
| 1:B:283:THR:OG1  | 1:B:372:ARG:HB2  | 2.20                     | 0.41              |
| 1:B:481:LEU:HD12 | 1:B:482:LEU:N    | 2.33                     | 0.41              |
| 1:B:724:MSE:O    | 1:B:728:VAL:HG23 | 2.20                     | 0.41              |
| 1:C:121:ASN:ND2  | 1:C:123:ARG:H    | 2.17                     | 0.41              |
| 1:C:168:ASP:O    | 1:C:174:TYR:HD2  | 2.03                     | 0.41              |
| 1:C:177:GLU:N    | 1:C:178:PRO:HD2  | 2.35                     | 0.41              |
| 1:C:190:LEU:O    | 1:C:196:GLN:HB2  | 2.19                     | 0.41              |
| 1:C:189:ARG:HA   | 1:C:202:PRO:HG3  | 2.02                     | 0.41              |
| 1:C:553:PRO:CG   | 1:C:620:VAL:HG21 | 2.50                     | 0.41              |
| 1:C:580:LYS:C    | 1:C:582:VAL:H    | 2.23                     | 0.41              |
| 1:D:128:PHE:CG   | 1:D:186:PRO:HG2  | 2.56                     | 0.41              |
| 1:D:168:ASP:O    | 1:D:174:TYR:HD2  | 2.03                     | 0.41              |
| 1:D:257:ILE:HD11 | 1:D:271:GLU:HG3  | 2.01                     | 0.41              |
| 1:D:474:ALA:C    | 1:D:476:GLU:H    | 2.23                     | 0.41              |
| 1:D:700:ARG:HD2  | 1:D:704:PHE:CE2  | 2.52                     | 0.41              |
| 1:E:18:ARG:HB2   | 1:E:19:PRO:CD    | 2.38                     | 0.41              |
| 1:E:18:ARG:HH12  | 1:E:36:ASN:ND2   | 2.19                     | 0.41              |
| 1:E:522:GLY:HA3  | 1:E:538:ILE:CD1  | 2.50                     | 0.41              |
| 1:E:526:TYR:CB   | 1:E:535:LEU:HD11 | 2.50                     | 0.41              |
| 1:E:739:THR:O    | 1:E:742:VAL:O    | 2.37                     | 0.41              |
| 1:F:312:THR:HA   | 1:F:315:ILE:HG22 | 2.02                     | 0.41              |
| 1:F:387:PHE:O    | 1:F:390:LEU:HG   | 2.20                     | 0.41              |
| 1:F:409:ASN:HD22 | 1:F:425:ILE:CD1  | 2.28                     | 0.41              |
| 1:A:86:PHE:O     | 1:A:88:ILE:HD12  | 2.19                     | 0.41              |
| 1:B:140:ILE:HB   | 1:B:152:THR:HG22 | 2.01                     | 0.41              |
| 1:B:19:PRO:HG3   | 1:B:174:TYR:O    | 2.19                     | 0.41              |
| 1:B:190:LEU:O    | 1:B:196:GLN:HB2  | 2.20                     | 0.41              |
| 1:B:21:VAL:HG11  | 1:B:44:ILE:HG21  | 2.02                     | 0.41              |
| 1:B:540:TYR:HD2  | 1:B:607:TYR:HB3  | 1.85                     | 0.41              |
| 1:C:148:ARG:NH2  | 1:C:158:MSE:N    | 2.68                     | 0.41              |
| 1:C:217:ALA:HB1  | 1:C:224:ILE:HD11 | 2.02                     | 0.41              |
| 1:C:472:GLU:O    | 1:C:476:GLU:HG2  | 2.20                     | 0.41              |
| 1:D:312:THR:HA   | 1:D:315:ILE:CG2  | 2.50                     | 0.41              |
| 1:E:106:ILE:HG22 | 1:E:107:ALA:N    | 2.35                     | 0.41              |
| 1:E:312:THR:CA   | 1:E:315:ILE:HG22 | 2.47                     | 0.41              |
| 1:E:410:ALA:HA   | 1:E:425:ILE:HD11 | 2.02                     | 0.41              |
| 1:E:7:HIS:CB     | 1:E:74:GLU:HB2   | 2.51                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:130:VAL:HG22 | 1:F:131:CYS:O    | 2.20                     | 0.41              |
| 1:F:247:GLN:OE1  | 1:F:637:LYS:HE3  | 2.21                     | 0.41              |
| 1:F:299:GLY:O    | 1:F:300:LEU:HG   | 2.20                     | 0.41              |
| 1:F:584:SER:HB3  | 1:F:589:LYS:HB3  | 2.02                     | 0.41              |
| 1:A:1:MSE:N      | 1:A:80:PRO:HD2   | 2.36                     | 0.41              |
| 1:A:1:MSE:HE3    | 1:A:2:LYS:H      | 1.85                     | 0.41              |
| 1:A:370:VAL:HG23 | 1:A:382:ARG:HB2  | 2.02                     | 0.41              |
| 1:A:504:ILE:HD12 | 1:A:701:ALA:CA   | 2.51                     | 0.41              |
| 1:A:487:HIS:CD2  | 1:A:520:TRP:HB3  | 2.56                     | 0.41              |
| 1:A:520:TRP:HZ2  | 1:A:534:ARG:HH21 | 1.68                     | 0.41              |
| 1:A:488:TYR:CD1  | 1:A:525:LEU:HD13 | 2.55                     | 0.41              |
| 1:B:161:PHE:O    | 1:B:164:SER:HB3  | 2.20                     | 0.41              |
| 1:B:258:GLU:O    | 1:B:261:LYS:N    | 2.52                     | 0.41              |
| 1:B:125:MSE:HE3  | 1:B:319:TRP:CH2  | 2.56                     | 0.41              |
| 1:B:321:LYS:HA   | 1:B:321:LYS:HD3  | 1.93                     | 0.41              |
| 1:B:582:VAL:HB   | 1:B:583:GLU:OE1  | 2.21                     | 0.41              |
| 1:B:558:MSE:HE1  | 1:B:593:ASN:ND2  | 2.36                     | 0.41              |
| 1:B:65:PRO:O     | 1:B:67:LEU:N     | 2.54                     | 0.41              |
| 1:C:493:SER:HB2  | 1:C:751:VAL:HG13 | 2.01                     | 0.41              |
| 1:D:248:LYS:HA   | 1:D:249:PRO:HD3  | 1.97                     | 0.41              |
| 1:D:219:LYS:HB2  | 1:D:357:LEU:HA   | 2.02                     | 0.41              |
| 1:E:493:SER:HB2  | 1:E:742:VAL:HG11 | 2.02                     | 0.41              |
| 1:E:55:ALA:O     | 1:E:59:ASP:HB2   | 2.19                     | 0.41              |
| 1:F:209:LEU:HA   | 1:F:212:LYS:CG   | 2.50                     | 0.41              |
| 1:F:38:GLY:HA2   | 1:F:144:LEU:HB3  | 2.02                     | 0.41              |
| 1:F:39:ASP:HB3   | 1:F:144:LEU:HD13 | 2.02                     | 0.41              |
| 1:F:415:LYS:O    | 1:F:416:ASN:HB2  | 2.20                     | 0.41              |
| 1:A:180:ALA:HB1  | 1:A:185:GLY:HA3  | 2.02                     | 0.41              |
| 1:A:456:ILE:HD12 | 1:A:456:ILE:N    | 2.36                     | 0.41              |
| 1:A:506:ILE:HD11 | 1:A:694:ALA:HA   | 2.02                     | 0.41              |
| 1:A:738:VAL:HG11 | 1:A:742:VAL:HG12 | 2.02                     | 0.41              |
| 1:B:18:ARG:N     | 1:B:19:PRO:CD    | 2.83                     | 0.41              |
| 1:B:368:ASP:HA   | 1:B:385:ARG:HD3  | 2.03                     | 0.41              |
| 1:B:383:ARG:CZ   | 1:B:387:PHE:HB3  | 2.50                     | 0.41              |
| 1:B:1:MSE:HB2    | 1:B:80:PRO:HD2   | 2.02                     | 0.41              |
| 1:C:123:ARG:NH2  | 1:C:173:ARG:NE   | 2.67                     | 0.41              |
| 1:C:292:LEU:HD12 | 1:C:296:LEU:CD2  | 2.47                     | 0.41              |
| 1:C:503:VAL:HA   | 1:C:706:VAL:HG11 | 2.03                     | 0.41              |
| 1:D:188:TYR:CD2  | 1:D:203:LEU:HD13 | 2.55                     | 0.41              |
| 1:D:236:VAL:HG21 | 1:D:296:LEU:HD12 | 2.03                     | 0.41              |
| 1:D:306:MSE:HE1  | 1:D:309:TYR:CE2  | 2.54                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:278:ARG:NH1  | 1:D:387:PHE:HE1  | 2.18                     | 0.41              |
| 1:D:595:VAL:O    | 1:D:598:GLN:HB3  | 2.20                     | 0.41              |
| 1:D:752:GLY:O    | 1:D:756:LEU:HD12 | 2.19                     | 0.41              |
| 1:E:130:VAL:HG21 | 1:E:135:GLY:HA3  | 2.03                     | 0.41              |
| 1:E:488:TYR:CD1  | 1:E:525:LEU:HD13 | 2.55                     | 0.41              |
| 1:E:700:ARG:HH11 | 1:E:704:PHE:HE2  | 1.67                     | 0.41              |
| 1:F:11:ILE:O     | 1:F:11:ILE:HG12  | 2.20                     | 0.41              |
| 1:F:186:PRO:HB3  | 1:F:359:ASN:HB2  | 2.03                     | 0.41              |
| 1:F:557:LEU:HD23 | 1:F:561:LEU:HD12 | 2.02                     | 0.41              |
| 1:F:620:VAL:HG22 | 1:F:625:ALA:O    | 2.20                     | 0.41              |
| 1:F:633:GLU:N    | 1:F:634:PRO:CD   | 2.81                     | 0.41              |
| 1:F:398:TYR:CE1  | 1:F:758:GLY:HA3  | 2.56                     | 0.41              |
| 1:A:132:THR:HG23 | 1:A:133:ASN:OD1  | 2.21                     | 0.41              |
| 1:A:286:LYS:HB2  | 1:A:303:ILE:CD1  | 2.51                     | 0.41              |
| 1:A:329:SER:CA   | 1:A:337:MSE:HE2  | 2.45                     | 0.41              |
| 1:A:399:ASN:HD22 | 1:A:399:ASN:N    | 2.19                     | 0.41              |
| 1:B:108:ILE:HG13 | 1:B:108:ILE:O    | 2.21                     | 0.41              |
| 1:B:116:LEU:HB3  | 1:B:129:ILE:HD13 | 2.03                     | 0.41              |
| 1:B:14:ALA:HA    | 1:B:146:TYR:CE1  | 2.56                     | 0.41              |
| 1:B:180:ALA:HB1  | 1:B:185:GLY:HA3  | 2.02                     | 0.41              |
| 1:B:265:TYR:HE2  | 1:B:287:LYS:CD   | 2.33                     | 0.41              |
| 1:B:508:LEU:HD11 | 1:B:725:ILE:CD1  | 2.51                     | 0.41              |
| 1:C:181:CYS:SG   | 1:C:182:PRO:HD2  | 2.60                     | 0.41              |
| 1:C:371:ILE:CB   | 1:C:380:VAL:HG13 | 2.49                     | 0.41              |
| 1:C:37:LEU:HB2   | 1:C:41:GLY:HA3   | 2.03                     | 0.41              |
| 1:D:261:LYS:HD3  | 1:D:266:VAL:HG21 | 2.03                     | 0.41              |
| 1:D:265:TYR:O    | 1:D:284:LEU:HD13 | 2.20                     | 0.41              |
| 1:D:290:PHE:HA   | 1:D:291:PRO:HD3  | 1.90                     | 0.41              |
| 1:D:493:SER:HB2  | 1:D:751:VAL:CG1  | 2.50                     | 0.41              |
| 1:E:498:LYS:CB   | 1:E:500:LEU:HD11 | 2.51                     | 0.41              |
| 1:E:501:ASP:O    | 1:E:503:VAL:HG13 | 2.20                     | 0.41              |
| 1:E:582:VAL:C    | 1:E:584:SER:H    | 2.23                     | 0.41              |
| 1:E:628:ARG:NH2  | 1:E:632:GLY:H    | 2.19                     | 0.41              |
| 1:E:12:VAL:CA    | 1:E:68:ALA:HB1   | 2.48                     | 0.41              |
| 1:F:111:ASP:HB2  | 1:F:172:ARG:NH2  | 2.27                     | 0.41              |
| 1:F:35:LYS:HG2   | 1:F:36:ASN:H     | 1.86                     | 0.41              |
| 1:C:591:GLU:HG3  | 1:F:471:MSE:O    | 2.20                     | 0.41              |
| 1:F:510:GLY:HA2  | 1:F:610:SER:OG   | 2.19                     | 0.41              |
| 1:F:522:GLY:HA3  | 1:F:611:THR:HG23 | 2.03                     | 0.41              |
| 1:A:738:VAL:HB   | 1:A:744:ARG:CG   | 2.51                     | 0.41              |
| 1:B:30:LEU:HD23  | 1:B:30:LEU:O     | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:370:VAL:HG23 | 1:B:381:ILE:CG1  | 2.51                     | 0.41              |
| 1:B:5:HIS:CD2    | 1:B:78:ILE:HD12  | 2.55                     | 0.41              |
| 1:C:171:ASN:HD21 | 1:C:173:ARG:HB2  | 1.82                     | 0.41              |
| 1:C:104:PRO:HB3  | 1:C:387:PHE:O    | 2.21                     | 0.41              |
| 1:D:502:SER:CB   | 1:D:528:GLY:HA2  | 2.48                     | 0.41              |
| 1:D:582:VAL:HG22 | 1:D:626:TYR:HB3  | 2.03                     | 0.41              |
| 1:E:612:GLY:O    | 1:E:615:LEU:HB2  | 2.20                     | 0.41              |
| 1:E:687:LEU:HD22 | 1:E:724:MSE:SE   | 2.70                     | 0.41              |
| 1:E:1:MSE:HB2    | 1:E:80:PRO:HD2   | 2.03                     | 0.41              |
| 1:F:140:ILE:HG21 | 1:F:360:ARG:HH11 | 1.85                     | 0.41              |
| 1:F:455:LEU:C    | 1:F:455:LEU:HD12 | 2.41                     | 0.41              |
| 1:F:474:ALA:C    | 1:F:476:GLU:H    | 2.22                     | 0.41              |
| 1:F:88:ILE:N     | 1:F:88:ILE:HD12  | 2.35                     | 0.41              |
| 1:A:264:ALA:O    | 1:A:265:TYR:HD2  | 2.03                     | 0.41              |
| 1:A:469:LEU:O    | 1:A:470:ALA:C    | 2.59                     | 0.41              |
| 1:A:472:GLU:HG3  | 1:A:473:MSE:N    | 2.36                     | 0.41              |
| 1:A:578:CYS:SG   | 1:A:578:CYS:O    | 2.79                     | 0.41              |
| 1:A:620:VAL:C    | 1:A:622:LEU:N    | 2.72                     | 0.41              |
| 1:A:691:ARG:HG3  | 1:A:724:MSE:HG3  | 2.03                     | 0.41              |
| 1:A:756:LEU:O    | 1:A:759:LEU:HB3  | 2.21                     | 0.41              |
| 1:B:202:PRO:O    | 1:B:203:LEU:C    | 2.58                     | 0.41              |
| 1:C:108:ILE:HG22 | 1:C:309:TYR:O    | 2.20                     | 0.41              |
| 1:C:413:VAL:CG2  | 1:C:448:LEU:HD12 | 2.51                     | 0.41              |
| 1:C:564:VAL:HG12 | 1:C:565:TYR:CD1  | 2.56                     | 0.41              |
| 1:D:279:ARG:HH11 | 1:D:279:ARG:HG3  | 1.85                     | 0.41              |
| 1:D:317:PHE:O    | 1:D:318:HIS:C    | 2.59                     | 0.41              |
| 1:D:383:ARG:HB3  | 1:D:747:ASN:ND2  | 2.34                     | 0.41              |
| 1:D:598:GLN:CG   | 1:D:604:ASN:HB2  | 2.50                     | 0.41              |
| 1:D:65:PRO:HG2   | 1:D:68:ALA:HB2   | 2.02                     | 0.41              |
| 1:D:66:PRO:HD3   | 1:D:133:ASN:HD22 | 1.86                     | 0.41              |
| 1:D:757:GLY:C    | 1:D:759:LEU:H    | 2.22                     | 0.41              |
| 1:E:142:GLU:HB3  | 1:E:150:ASN:C    | 2.41                     | 0.41              |
| 1:E:219:LYS:HA   | 1:E:224:ILE:CB   | 2.51                     | 0.41              |
| 1:E:461:HIS:CE1  | 1:E:463:ALA:HB3  | 2.56                     | 0.41              |
| 1:F:621:LEU:O    | 1:F:622:LEU:HD23 | 2.21                     | 0.41              |
| 1:A:111:ASP:HB2  | 1:A:172:ARG:HH22 | 1.86                     | 0.41              |
| 1:A:339:LYS:HG3  | 1:A:365:ARG:HH12 | 1.84                     | 0.41              |
| 1:A:376:GLY:HA2  | 1:A:726:ARG:NH1  | 2.35                     | 0.41              |
| 1:A:456:ILE:HD12 | 1:A:480:GLU:O    | 2.20                     | 0.41              |
| 1:A:613:ARG:O    | 1:A:616:ASP:HB3  | 2.21                     | 0.41              |
| 1:A:535:LEU:HD23 | 1:A:700:ARG:HG3  | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:737:HIS:HD2  | 1:A:744:ARG:NE   | 2.19                     | 0.41              |
| 1:B:102:ILE:HA   | 1:B:102:ILE:HD13 | 1.91                     | 0.41              |
| 1:B:171:ASN:ND2  | 1:B:173:ARG:CB   | 2.84                     | 0.41              |
| 1:B:190:LEU:HB2  | 1:B:202:PRO:HB3  | 2.02                     | 0.41              |
| 1:B:482:LEU:HD12 | 1:B:483:GLN:N    | 2.35                     | 0.41              |
| 1:B:619:ALA:HB1  | 1:B:625:ALA:CB   | 2.50                     | 0.41              |
| 1:B:656:GLU:HG3  | 1:B:661:ARG:CZ   | 2.51                     | 0.41              |
| 1:C:12:VAL:HG13  | 1:C:13:GLN:N     | 2.32                     | 0.41              |
| 1:C:154:LYS:O    | 1:C:154:LYS:HD3  | 2.21                     | 0.41              |
| 1:C:204:ARG:HG2  | 1:C:319:TRP:CE2  | 2.56                     | 0.41              |
| 1:C:253:MSE:HE1  | 1:C:313:HIS:CG   | 2.56                     | 0.41              |
| 1:C:309:TYR:CZ   | 1:C:385:ARG:NH1  | 2.83                     | 0.41              |
| 1:C:341:ASN:O    | 1:C:344:ALA:HB3  | 2.21                     | 0.41              |
| 1:C:601:LYS:HB3  | 1:C:603:ILE:HG13 | 2.03                     | 0.41              |
| 1:D:233:GLU:HA   | 1:D:236:VAL:CG1  | 2.50                     | 0.41              |
| 1:D:247:GLN:HG3  | 1:D:298:PRO:CG   | 2.38                     | 0.41              |
| 1:D:348:LEU:N    | 1:D:348:LEU:HD12 | 2.36                     | 0.41              |
| 1:D:422:SER:HA   | 1:D:444:PHE:CZ   | 2.56                     | 0.41              |
| 1:D:695:HIS:CE1  | 1:D:728:VAL:HG13 | 2.55                     | 0.41              |
| 1:D:760:TYR:CE2  | 1:D:767:LYS:HG2  | 2.53                     | 0.41              |
| 1:F:220:GLY:H    | 1:F:224:ILE:HA   | 1.85                     | 0.41              |
| 1:F:270:GLU:CA   | 1:F:373:PHE:HE2  | 2.34                     | 0.41              |
| 1:F:596:LEU:O    | 1:F:600:ALA:N    | 2.54                     | 0.41              |
| 1:F:601:LYS:HD2  | 1:F:603:ILE:HD11 | 2.03                     | 0.41              |
| 1:A:409:ASN:CG   | 1:A:410:ALA:H    | 2.24                     | 0.41              |
| 1:A:413:VAL:HG13 | 1:A:420:TYR:HB2  | 2.02                     | 0.41              |
| 1:A:504:ILE:HG22 | 1:A:505:GLY:N    | 2.35                     | 0.41              |
| 1:A:528:GLY:O    | 1:A:529:TYR:C    | 2.59                     | 0.41              |
| 1:A:587:TYR:CD1  | 1:A:588:GLY:N    | 2.74                     | 0.41              |
| 1:B:250:PHE:O    | 1:B:252:ILE:HD12 | 2.21                     | 0.41              |
| 1:B:256:ASP:O    | 1:B:257:ILE:C    | 2.59                     | 0.41              |
| 1:B:286:LYS:HB2  | 1:B:303:ILE:CD1  | 2.51                     | 0.41              |
| 1:B:252:ILE:CD1  | 1:B:296:LEU:HD23 | 2.51                     | 0.41              |
| 1:B:221:ILE:HD11 | 1:B:309:TYR:CE1  | 2.56                     | 0.41              |
| 1:B:21:VAL:CG1   | 1:B:44:ILE:HD13  | 2.51                     | 0.41              |
| 1:B:639:GLU:OE2  | 1:B:718:ASN:HA   | 2.21                     | 0.41              |
| 1:C:102:ILE:CD1  | 1:C:144:LEU:HG   | 2.51                     | 0.41              |
| 1:C:534:ARG:C    | 1:C:535:LEU:HD12 | 2.41                     | 0.41              |
| 1:C:601:LYS:CB   | 1:C:603:ILE:HG13 | 2.51                     | 0.41              |
| 1:D:134:CYS:SG   | 1:D:135:GLY:N    | 2.93                     | 0.41              |
| 1:D:203:LEU:HD21 | 1:D:315:ILE:CG2  | 2.51                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:427:ASN:O    | 1:D:433:VAL:HG11 | 2.21                     | 0.41              |
| 1:D:447:ILE:O    | 1:D:448:LEU:HD23 | 2.21                     | 0.41              |
| 1:D:451:LYS:O    | 1:D:451:LYS:HG3  | 2.21                     | 0.41              |
| 1:E:22:TYR:CE1   | 1:E:87:TYR:HB3   | 2.56                     | 0.41              |
| 1:E:288:GLU:HB3  | 1:E:289:PRO:CD   | 2.38                     | 0.41              |
| 1:E:653:VAL:O    | 1:E:653:VAL:HG13 | 2.21                     | 0.41              |
| 1:E:688:ALA:O    | 1:E:691:ARG:HB3  | 2.21                     | 0.41              |
| 1:E:690:ALA:HB2  | 1:E:721:ILE:HG12 | 2.03                     | 0.41              |
| 1:F:137:ARG:NH2  | 1:F:178:PRO:HG3  | 2.31                     | 0.41              |
| 1:F:552:TYR:O    | 1:F:555:ARG:HG3  | 2.20                     | 0.41              |
| 1:F:64:LYS:CB    | 1:F:65:PRO:HD2   | 2.51                     | 0.41              |
| 1:A:286:LYS:HD2  | 1:A:303:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:399:ASN:N    | 1:A:454:ASP:OD1  | 2.54                     | 0.41              |
| 1:A:618:ILE:HG22 | 1:A:638:LEU:HD21 | 2.03                     | 0.41              |
| 1:B:15:VAL:HG21  | 1:B:68:ALA:HB2   | 2.03                     | 0.41              |
| 1:B:20:PHE:HE1   | 1:B:60:LEU:HA    | 1.86                     | 0.41              |
| 1:B:309:TYR:C    | 1:B:309:TYR:CD1  | 2.94                     | 0.41              |
| 1:B:373:PHE:CZ   | 1:B:378:ARG:HD3  | 2.55                     | 0.41              |
| 1:B:42:VAL:HG22  | 1:B:42:VAL:O     | 2.21                     | 0.41              |
| 1:B:497:GLU:OE1  | 1:B:738:VAL:HA   | 2.21                     | 0.41              |
| 1:B:598:GLN:HG3  | 1:B:604:ASN:HB2  | 2.03                     | 0.41              |
| 1:B:626:TYR:C    | 1:B:627:ARG:HG2  | 2.40                     | 0.41              |
| 1:B:761:LEU:O    | 1:B:761:LEU:HD12 | 2.20                     | 0.41              |
| 1:C:320:SER:O    | 1:C:321:LYS:C    | 2.58                     | 0.41              |
| 1:C:494:VAL:HG11 | 1:C:710:ALA:HB1  | 2.02                     | 0.41              |
| 1:C:526:TYR:HB2  | 1:C:535:LEU:HD11 | 2.03                     | 0.41              |
| 1:C:554:LEU:HD23 | 1:C:583:GLU:OE2  | 2.21                     | 0.41              |
| 1:C:404:GLY:HA2  | 1:C:753:GLN:OE1  | 2.21                     | 0.41              |
| 1:D:148:ARG:CZ   | 1:D:158:MSE:HG3  | 2.51                     | 0.41              |
| 1:D:177:GLU:N    | 1:D:178:PRO:HD2  | 2.36                     | 0.41              |
| 1:D:147:ASP:HA   | 1:D:177:GLU:OE2  | 2.21                     | 0.41              |
| 1:D:339:LYS:O    | 1:D:340:ASP:C    | 2.59                     | 0.41              |
| 1:D:557:LEU:O    | 1:D:561:LEU:HG   | 2.21                     | 0.41              |
| 1:D:694:ALA:O    | 1:D:698:VAL:HG23 | 2.20                     | 0.41              |
| 1:E:13:GLN:NE2   | 1:E:18:ARG:NH2   | 2.69                     | 0.41              |
| 1:E:198:ILE:O    | 1:E:199:TYR:HB3  | 2.21                     | 0.41              |
| 1:E:433:VAL:O    | 1:E:436:PHE:N    | 2.52                     | 0.41              |
| 1:E:8:VAL:O      | 1:E:42:VAL:HB    | 2.21                     | 0.41              |
| 1:F:153:MSE:HA   | 1:F:156:PHE:HD2  | 1.86                     | 0.41              |
| 1:F:500:LEU:HD12 | 1:F:501:ASP:O    | 2.21                     | 0.41              |
| 1:A:252:ILE:HD13 | 1:A:303:ILE:CG2  | 2.51                     | 0.40              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:496:ALA:HB2  | 1:A:755:PHE:CD2  | 2.56                     | 0.40              |
| 1:A:50:GLU:O     | 1:A:53:ILE:HG22  | 2.21                     | 0.40              |
| 1:A:630:TYR:HD1  | 1:A:631:GLU:N    | 2.19                     | 0.40              |
| 1:B:460:LEU:CD2  | 1:B:515:THR:HG22 | 2.51                     | 0.40              |
| 1:B:524:VAL:CG2  | 1:B:536:ALA:HB3  | 2.47                     | 0.40              |
| 1:C:406:GLU:HA   | 1:C:466:THR:HG21 | 2.03                     | 0.40              |
| 1:C:543:LEU:HD12 | 1:C:549:ALA:CB   | 2.51                     | 0.40              |
| 1:C:31:ARG:HG2   | 1:C:85:ARG:C     | 2.42                     | 0.40              |
| 1:D:170:LEU:H    | 1:D:170:LEU:CD1  | 2.29                     | 0.40              |
| 1:D:171:ASN:HD21 | 1:D:173:ARG:HB2  | 1.86                     | 0.40              |
| 1:D:205:LYS:HE3  | 1:D:205:LYS:HB2  | 1.84                     | 0.40              |
| 1:D:522:GLY:H    | 1:D:523:GLU:CD   | 2.23                     | 0.40              |
| 1:E:209:LEU:O    | 1:E:212:LYS:HB2  | 2.20                     | 0.40              |
| 1:E:218:ILE:HD12 | 1:E:356:LEU:CD2  | 2.51                     | 0.40              |
| 1:E:66:PRO:HD2   | 1:E:133:ASN:HD21 | 1.85                     | 0.40              |
| 1:E:739:THR:O    | 1:E:740:THR:C    | 2.60                     | 0.40              |
| 1:F:249:PRO:CG   | 1:F:300:LEU:HD13 | 2.45                     | 0.40              |
| 1:F:552:TYR:HA   | 1:F:553:PRO:HD2  | 1.89                     | 0.40              |
| 1:F:615:LEU:HD23 | 1:F:635:ALA:CB   | 2.52                     | 0.40              |
| 1:A:148:ARG:C    | 1:A:150:ASN:H    | 2.25                     | 0.40              |
| 1:A:307:LEU:HB3  | 1:A:308:PRO:HD2  | 2.01                     | 0.40              |
| 1:A:38:GLY:C     | 1:A:40:ALA:N     | 2.74                     | 0.40              |
| 1:A:398:TYR:CG   | 1:A:398:TYR:O    | 2.74                     | 0.40              |
| 1:A:683:TYR:O    | 1:A:687:LEU:HG   | 2.22                     | 0.40              |
| 1:A:694:ALA:O    | 1:A:697:ALA:N    | 2.54                     | 0.40              |
| 1:B:332:TYR:HB3  | 1:B:333:PRO:HD2  | 2.03                     | 0.40              |
| 1:B:224:ILE:HG12 | 1:B:338:VAL:HG13 | 2.03                     | 0.40              |
| 1:B:242:ARG:HD3  | 1:B:351:VAL:O    | 2.21                     | 0.40              |
| 1:B:365:ARG:O    | 1:B:366:ALA:HB2  | 2.21                     | 0.40              |
| 1:B:413:VAL:HG11 | 1:B:448:LEU:HD11 | 2.03                     | 0.40              |
| 1:B:525:LEU:CA   | 1:B:535:LEU:HD13 | 2.51                     | 0.40              |
| 1:B:616:ASP:O    | 1:B:619:ALA:HB3  | 2.21                     | 0.40              |
| 1:B:15:VAL:HG11  | 1:B:67:LEU:HB2   | 2.02                     | 0.40              |
| 1:C:142:GLU:O    | 1:C:143:ASP:HB2  | 2.20                     | 0.40              |
| 1:C:282:ILE:HA   | 1:C:371:ILE:O    | 2.22                     | 0.40              |
| 1:C:370:VAL:HG23 | 1:C:381:ILE:CD1  | 2.51                     | 0.40              |
| 1:C:6:ILE:HG13   | 1:C:57:ILE:HD11  | 2.04                     | 0.40              |
| 1:D:163:ARG:CB   | 1:D:163:ARG:HH11 | 2.32                     | 0.40              |
| 1:D:279:ARG:CG   | 1:D:279:ARG:HH11 | 2.34                     | 0.40              |
| 1:D:453:LEU:HG   | 1:D:453:LEU:O    | 2.21                     | 0.40              |
| 1:D:649:LEU:HD23 | 1:D:651:PHE:HE1  | 1.86                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:279:ARG:N    | 1:E:280:PRO:CD   | 2.84                     | 0.40              |
| 1:E:383:ARG:O    | 1:E:384:SER:HB3  | 2.21                     | 0.40              |
| 1:E:34:VAL:O     | 1:E:89:GLU:HA    | 2.21                     | 0.40              |
| 1:F:451:LYS:O    | 1:F:451:LYS:HG3  | 2.22                     | 0.40              |
| 1:F:553:PRO:HG3  | 1:F:626:TYR:O    | 2.21                     | 0.40              |
| 1:F:743:PRO:HG2  | 1:F:748:GLY:CA   | 2.49                     | 0.40              |
| 1:A:108:ILE:HG13 | 1:A:311:GLY:N    | 2.32                     | 0.40              |
| 1:A:561:LEU:HB3  | 1:A:570:LEU:HD13 | 2.02                     | 0.40              |
| 1:A:642:ALA:HB1  | 1:A:683:TYR:HA   | 2.03                     | 0.40              |
| 1:B:253:MSE:HE2  | 1:B:317:PHE:HD1  | 1.86                     | 0.40              |
| 1:B:278:ARG:O    | 1:B:279:ARG:C    | 2.60                     | 0.40              |
| 1:B:303:ILE:HG22 | 1:B:304:GLY:N    | 2.36                     | 0.40              |
| 1:C:172:ARG:HG2  | 1:C:173:ARG:HD3  | 2.03                     | 0.40              |
| 1:D:210:ILE:HD13 | 1:D:216:VAL:CG1  | 2.47                     | 0.40              |
| 1:D:292:LEU:HD11 | 1:D:324:VAL:HG21 | 2.02                     | 0.40              |
| 1:D:35:LYS:O     | 1:D:42:VAL:HG13  | 2.22                     | 0.40              |
| 1:D:383:ARG:HG3  | 1:D:383:ARG:NH1  | 2.37                     | 0.40              |
| 1:D:104:PRO:HD3  | 1:D:390:LEU:HD21 | 2.04                     | 0.40              |
| 1:D:437:MSE:HE1  | 1:D:466:THR:HG22 | 2.03                     | 0.40              |
| 1:D:727:LYS:HA   | 1:D:730:GLU:HG2  | 2.03                     | 0.40              |
| 1:D:497:GLU:OE2  | 1:D:738:VAL:HG12 | 2.22                     | 0.40              |
| 1:E:140:ILE:HB   | 1:E:152:THR:CG2  | 2.51                     | 0.40              |
| 1:E:252:ILE:CG2  | 1:E:324:VAL:HB   | 2.51                     | 0.40              |
| 1:E:415:LYS:O    | 1:E:417:GLY:N    | 2.54                     | 0.40              |
| 1:E:73:ILE:O     | 1:E:73:ILE:HG22  | 2.21                     | 0.40              |
| 1:F:270:GLU:CB   | 1:F:373:PHE:HE2  | 2.34                     | 0.40              |
| 1:F:394:ILE:HG23 | 1:F:755:PHE:HB2  | 2.04                     | 0.40              |
| 1:F:532:VAL:HG12 | 1:F:533:GLU:N    | 2.37                     | 0.40              |
| 1:F:582:VAL:O    | 1:F:627:ARG:HD2  | 2.21                     | 0.40              |
| 1:F:722:THR:O    | 1:F:722:THR:HG22 | 2.22                     | 0.40              |
| 1:A:116:LEU:HD12 | 1:A:116:LEU:C    | 2.42                     | 0.40              |
| 1:A:154:LYS:HD3  | 1:A:154:LYS:C    | 2.42                     | 0.40              |
| 1:A:207:ALA:C    | 1:A:209:LEU:N    | 2.75                     | 0.40              |
| 1:A:219:LYS:HB2  | 1:A:357:LEU:HA   | 2.03                     | 0.40              |
| 1:A:21:VAL:HA    | 1:A:24:ILE:CG2   | 2.52                     | 0.40              |
| 1:A:228:CYS:O    | 1:A:326:VAL:HB   | 2.22                     | 0.40              |
| 1:A:457:ILE:HA   | 1:A:482:LEU:O    | 2.21                     | 0.40              |
| 1:A:561:LEU:HD22 | 1:A:565:TYR:CE2  | 2.57                     | 0.40              |
| 1:A:588:GLY:O    | 1:A:592:PHE:CD2  | 2.75                     | 0.40              |
| 1:B:207:ALA:HB1  | 1:B:320:SER:CB   | 2.52                     | 0.40              |
| 1:B:217:ALA:HA   | 1:B:226:LEU:HA   | 2.02                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:259:THR:O    | 1:B:263:PHE:HB2  | 2.22                     | 0.40              |
| 1:B:278:ARG:HG3  | 1:B:280:PRO:HD3  | 2.03                     | 0.40              |
| 1:B:253:MSE:HA   | 1:B:306:MSE:HB2  | 2.04                     | 0.40              |
| 1:B:582:VAL:HG11 | 1:B:626:TYR:HB3  | 2.04                     | 0.40              |
| 1:C:106:ILE:HG12 | 1:C:277:TYR:CD1  | 2.56                     | 0.40              |
| 1:C:312:THR:HA   | 1:C:315:ILE:CG2  | 2.49                     | 0.40              |
| 1:C:737:HIS:O    | 1:C:738:VAL:C    | 2.58                     | 0.40              |
| 1:C:424:TYR:HD1  | 1:C:747:ASN:HD22 | 1.68                     | 0.40              |
| 1:D:125:MSE:HE3  | 1:D:319:TRP:CH2  | 2.56                     | 0.40              |
| 1:D:152:THR:HG23 | 1:D:153:MSE:N    | 2.36                     | 0.40              |
| 1:D:219:LYS:HG2  | 1:D:358:HIS:CE1  | 2.55                     | 0.40              |
| 1:D:729:VAL:O    | 1:D:729:VAL:HG12 | 2.21                     | 0.40              |
| 1:E:11:ILE:O     | 1:E:13:GLN:N     | 2.55                     | 0.40              |
| 1:E:239:LEU:HD22 | 1:E:250:PHE:CZ   | 2.56                     | 0.40              |
| 1:E:261:LYS:HD3  | 1:E:266:VAL:CG2  | 2.51                     | 0.40              |
| 1:E:459:ASP:C    | 1:E:461:HIS:H    | 2.25                     | 0.40              |
| 1:E:406:GLU:HB3  | 1:E:464:TYR:CD2  | 2.56                     | 0.40              |
| 1:F:413:VAL:CG2  | 1:F:448:LEU:HD13 | 2.48                     | 0.40              |
| 1:F:614:VAL:HG11 | 1:F:662:VAL:HG11 | 2.03                     | 0.40              |
| 1:F:771:MSE:O    | 1:F:772:LEU:HD23 | 2.21                     | 0.40              |
| 1:A:105:ASP:OD1  | 1:A:139:THR:HG23 | 2.22                     | 0.40              |
| 1:A:12:VAL:HG12  | 1:A:13:GLN:N     | 2.37                     | 0.40              |
| 1:A:196:GLN:HE21 | 1:A:196:GLN:N    | 2.19                     | 0.40              |
| 1:A:90:LYS:HB3   | 1:A:90:LYS:HE2   | 1.93                     | 0.40              |
| 1:B:228:CYS:O    | 1:B:326:VAL:HG23 | 2.21                     | 0.40              |
| 1:B:248:LYS:HA   | 1:B:249:PRO:HD3  | 1.97                     | 0.40              |
| 1:B:153:MSE:HE1  | 1:B:360:ARG:NE   | 2.36                     | 0.40              |
| 1:C:128:PHE:CE1  | 1:C:186:PRO:HG2  | 2.57                     | 0.40              |
| 1:C:394:ILE:HD11 | 1:C:419:VAL:CG1  | 2.51                     | 0.40              |
| 1:C:516:ASP:HB2  | 1:C:518:ASN:HD22 | 1.84                     | 0.40              |
| 1:C:555:ARG:NH1  | 1:C:592:PHE:CE1  | 2.90                     | 0.40              |
| 1:C:618:ILE:H    | 1:C:618:ILE:HG13 | 1.71                     | 0.40              |
| 1:D:394:ILE:HG23 | 1:D:395:PRO:HD2  | 2.02                     | 0.40              |
| 1:D:395:PRO:HG2  | 1:D:396:PHE:CE2  | 2.55                     | 0.40              |
| 1:D:506:ILE:HG23 | 1:D:693:PHE:CE1  | 2.57                     | 0.40              |
| 1:D:543:LEU:HB2  | 1:D:549:ALA:CB   | 2.52                     | 0.40              |
| 1:D:612:GLY:O    | 1:D:615:LEU:HB2  | 2.22                     | 0.40              |
| 1:D:6:ILE:O      | 1:D:43:GLU:HA    | 2.22                     | 0.40              |
| 1:E:278:ARG:HG2  | 1:E:278:ARG:H    | 1.72                     | 0.40              |
| 1:E:399:ASN:HA   | 1:E:414:ALA:O    | 2.22                     | 0.40              |
| 1:F:413:VAL:HG11 | 1:F:448:LEU:CD1  | 2.52                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:524:VAL:HG23 | 1:F:536:ALA:H    | 1.86                     | 0.40              |
| 1:F:557:LEU:HD11 | 1:F:621:LEU:CA   | 2.50                     | 0.40              |
| 1:F:601:LYS:CD   | 1:F:603:ILE:HD11 | 2.51                     | 0.40              |
| 1:F:620:VAL:HG13 | 1:F:626:TYR:CE1  | 2.57                     | 0.40              |
| 1:F:8:VAL:O      | 1:F:9:GLN:HG3    | 2.22                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------------|--------------------------|-------------------|
| 1:A:204:ARG:NH1 | 1:A:204:ARG:NH1[12_554] | 1.95                     | 0.25              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 762/772 (99%)   | 530 (70%)  | 179 (24%) | 53 (7%)  | 1           | 17 |
| 1   | B     | 758/772 (98%)   | 565 (74%)  | 145 (19%) | 48 (6%)  | 1           | 19 |
| 1   | C     | 750/772 (97%)   | 540 (72%)  | 170 (23%) | 40 (5%)  | 2           | 22 |
| 1   | D     | 761/772 (99%)   | 580 (76%)  | 148 (19%) | 33 (4%)  | 2           | 25 |
| 1   | E     | 758/772 (98%)   | 566 (75%)  | 149 (20%) | 43 (6%)  | 1           | 20 |
| 1   | F     | 758/772 (98%)   | 562 (74%)  | 171 (23%) | 25 (3%)  | 4           | 30 |
| All | All   | 4547/4632 (98%) | 3343 (74%) | 962 (21%) | 242 (5%) | 2           | 22 |

All (242) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 194 | ASP  |
| 1   | A     | 203 | LEU  |
| 1   | A     | 264 | ALA  |

Continued on next page...

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 311        | GLY         |
| 1          | B            | 42         | VAL         |
| 1          | B            | 625        | ALA         |
| 1          | C            | 255        | LYS         |
| 1          | C            | 291        | PRO         |
| 1          | C            | 323        | PRO         |
| 1          | C            | 363        | LEU         |
| 1          | C            | 624        | VAL         |
| 1          | D            | 11         | ILE         |
| 1          | D            | 321        | LYS         |
| 1          | D            | 384        | SER         |
| 1          | D            | 603        | ILE         |
| 1          | D            | 738        | VAL         |
| 1          | E            | 255        | LYS         |
| 1          | E            | 384        | SER         |
| 1          | E            | 624        | VAL         |
| 1          | F            | 194        | ASP         |
| 1          | F            | 202        | PRO         |
| 1          | F            | 203        | LEU         |
| 1          | F            | 321        | LYS         |
| 1          | F            | 603        | ILE         |
| 1          | F            | 738        | VAL         |
| 1          | A            | 13         | GLN         |
| 1          | A            | 202        | PRO         |
| 1          | A            | 268        | PRO         |
| 1          | A            | 291        | PRO         |
| 1          | A            | 321        | LYS         |
| 1          | A            | 323        | PRO         |
| 1          | A            | 351        | VAL         |
| 1          | A            | 384        | SER         |
| 1          | A            | 428        | THR         |
| 1          | A            | 429        | GLY         |
| 1          | A            | 499        | ASN         |
| 1          | A            | 603        | ILE         |
| 1          | A            | 609        | SER         |
| 1          | A            | 624        | VAL         |
| 1          | A            | 725        | ILE         |
| 1          | B            | 291        | PRO         |
| 1          | B            | 320        | SER         |
| 1          | B            | 323        | PRO         |
| 1          | B            | 366        | ALA         |
| 1          | B            | 455        | LEU         |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 529        | TYR         |
| 1          | B            | 741        | GLU         |
| 1          | C            | 41         | GLY         |
| 1          | C            | 321        | LYS         |
| 1          | C            | 362        | ILE         |
| 1          | C            | 384        | SER         |
| 1          | C            | 531        | ASP         |
| 1          | C            | 586        | LYS         |
| 1          | C            | 718        | ASN         |
| 1          | D            | 13         | GLN         |
| 1          | D            | 194        | ASP         |
| 1          | D            | 319        | TRP         |
| 1          | D            | 632        | GLY         |
| 1          | D            | 644        | LYS         |
| 1          | D            | 715        | VAL         |
| 1          | E            | 194        | ASP         |
| 1          | E            | 203        | LEU         |
| 1          | E            | 319        | TRP         |
| 1          | E            | 320        | SER         |
| 1          | E            | 429        | GLY         |
| 1          | E            | 495        | MSE         |
| 1          | E            | 603        | ILE         |
| 1          | E            | 632        | GLY         |
| 1          | E            | 715        | VAL         |
| 1          | E            | 738        | VAL         |
| 1          | F            | 291        | PRO         |
| 1          | F            | 363        | LEU         |
| 1          | F            | 384        | SER         |
| 1          | F            | 545        | GLY         |
| 1          | A            | 130        | VAL         |
| 1          | A            | 255        | LYS         |
| 1          | A            | 329        | SER         |
| 1          | A            | 363        | LEU         |
| 1          | A            | 424        | TYR         |
| 1          | A            | 657        | GLY         |
| 1          | A            | 714        | GLY         |
| 1          | A            | 715        | VAL         |
| 1          | A            | 732        | ASN         |
| 1          | B            | 81         | GLN         |
| 1          | B            | 83         | PHE         |
| 1          | B            | 194        | ASP         |
| 1          | B            | 268        | PRO         |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 321        | LYS         |
| 1          | B            | 360        | ARG         |
| 1          | B            | 384        | SER         |
| 1          | B            | 715        | VAL         |
| 1          | B            | 738        | VAL         |
| 1          | C            | 29         | ASN         |
| 1          | C            | 234        | GLU         |
| 1          | C            | 360        | ARG         |
| 1          | C            | 423        | GLN         |
| 1          | C            | 539        | ASP         |
| 1          | C            | 609        | SER         |
| 1          | C            | 738        | VAL         |
| 1          | D            | 49         | ARG         |
| 1          | D            | 143        | ASP         |
| 1          | D            | 291        | PRO         |
| 1          | D            | 320        | SER         |
| 1          | D            | 323        | PRO         |
| 1          | E            | 12         | VAL         |
| 1          | E            | 83         | PHE         |
| 1          | E            | 199        | TYR         |
| 1          | E            | 202        | PRO         |
| 1          | E            | 268        | PRO         |
| 1          | E            | 291        | PRO         |
| 1          | E            | 586        | LYS         |
| 1          | E            | 648        | ASP         |
| 1          | E            | 718        | ASN         |
| 1          | F            | 715        | VAL         |
| 1          | A            | 113        | LEU         |
| 1          | A            | 502        | SER         |
| 1          | A            | 516        | ASP         |
| 1          | A            | 539        | ASP         |
| 1          | A            | 551        | TYR         |
| 1          | B            | 12         | VAL         |
| 1          | B            | 143        | ASP         |
| 1          | B            | 247        | GLN         |
| 1          | B            | 255        | LYS         |
| 1          | B            | 330        | ALA         |
| 1          | B            | 521        | GLY         |
| 1          | B            | 609        | SER         |
| 1          | C            | 143        | ASP         |
| 1          | C            | 361        | LYS         |
| 1          | C            | 521        | GLY         |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | C            | 729        | VAL         |
| 1          | D            | 268        | PRO         |
| 1          | D            | 339        | LYS         |
| 1          | D            | 346        | GLU         |
| 1          | D            | 586        | LYS         |
| 1          | E            | 63         | LYS         |
| 1          | E            | 323        | PRO         |
| 1          | E            | 410        | ALA         |
| 1          | E            | 460        | LEU         |
| 1          | E            | 741        | GLU         |
| 1          | F            | 63         | LYS         |
| 1          | F            | 83         | PHE         |
| 1          | F            | 540        | TYR         |
| 1          | F            | 648        | ASP         |
| 1          | F            | 695        | HIS         |
| 1          | A            | 117        | PHE         |
| 1          | A            | 214        | TYR         |
| 1          | A            | 416        | ASN         |
| 1          | A            | 425        | ILE         |
| 1          | A            | 453        | LEU         |
| 1          | A            | 514        | GLY         |
| 1          | A            | 581        | ALA         |
| 1          | A            | 667        | GLN         |
| 1          | A            | 718        | ASN         |
| 1          | B            | 66         | PRO         |
| 1          | B            | 296        | LEU         |
| 1          | B            | 311        | GLY         |
| 1          | B            | 333        | PRO         |
| 1          | B            | 460        | LEU         |
| 1          | B            | 499        | ASN         |
| 1          | B            | 514        | GLY         |
| 1          | B            | 623        | ASN         |
| 1          | B            | 630        | TYR         |
| 1          | B            | 678        | PRO         |
| 1          | C            | 36         | ASN         |
| 1          | C            | 88         | ILE         |
| 1          | C            | 324        | VAL         |
| 1          | C            | 499        | ASN         |
| 1          | C            | 603        | ILE         |
| 1          | C            | 652        | GLU         |
| 1          | D            | 130        | VAL         |
| 1          | D            | 180        | ALA         |

*Continued on next page...*



*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | D            | 424        | TYR         |
| 1          | E            | 15         | VAL         |
| 1          | E            | 36         | ASN         |
| 1          | E            | 66         | PRO         |
| 1          | E            | 127        | PRO         |
| 1          | E            | 416        | ASN         |
| 1          | E            | 678        | PRO         |
| 1          | F            | 6          | ILE         |
| 1          | F            | 234        | GLU         |
| 1          | F            | 514        | GLY         |
| 1          | F            | 521        | GLY         |
| 1          | A            | 12         | VAL         |
| 1          | A            | 143        | ASP         |
| 1          | A            | 405        | ALA         |
| 1          | A            | 521        | GLY         |
| 1          | B            | 137        | ARG         |
| 1          | B            | 633        | GLU         |
| 1          | C            | 268        | PRO         |
| 1          | C            | 567        | ILE         |
| 1          | D            | 329        | SER         |
| 1          | D            | 425        | ILE         |
| 1          | D            | 741        | GLU         |
| 1          | F            | 632        | GLY         |
| 1          | A            | 249        | PRO         |
| 1          | B            | 82         | GLY         |
| 1          | B            | 130        | VAL         |
| 1          | B            | 511        | VAL         |
| 1          | C            | 715        | VAL         |
| 1          | E            | 73         | ILE         |
| 1          | E            | 426        | GLY         |
| 1          | F            | 15         | VAL         |
| 1          | F            | 323        | PRO         |
| 1          | A            | 326        | VAL         |
| 1          | A            | 738        | VAL         |
| 1          | B            | 362        | ILE         |
| 1          | B            | 517        | GLY         |
| 1          | B            | 522        | GLY         |
| 1          | C            | 11         | ILE         |
| 1          | C            | 45         | VAL         |
| 1          | D            | 66         | PRO         |
| 1          | D            | 333        | PRO         |
| 1          | A            | 511        | VAL         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 634 | PRO  |
| 1   | B     | 202 | PRO  |
| 1   | B     | 603 | ILE  |
| 1   | B     | 705 | GLY  |
| 1   | D     | 429 | GLY  |
| 1   | E     | 521 | GLY  |
| 1   | F     | 324 | VAL  |
| 1   | A     | 41  | GLY  |
| 1   | C     | 127 | PRO  |
| 1   | C     | 202 | PRO  |
| 1   | C     | 257 | ILE  |
| 1   | D     | 41  | GLY  |
| 1   | D     | 73  | ILE  |
| 1   | D     | 403 | VAL  |
| 1   | E     | 333 | PRO  |
| 1   | E     | 351 | VAL  |
| 1   | E     | 425 | ILE  |
| 1   | F     | 511 | VAL  |
| 1   | A     | 698 | VAL  |
| 1   | B     | 257 | ILE  |
| 1   | B     | 729 | VAL  |
| 1   | C     | 130 | VAL  |
| 1   | C     | 511 | VAL  |
| 1   | E     | 186 | PRO  |
| 1   | E     | 249 | PRO  |
| 1   | E     | 311 | GLY  |
| 1   | E     | 389 | PRO  |
| 1   | D     | 389 | PRO  |
| 1   | C     | 389 | PRO  |

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

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles        |
|-----|-------|----------------|-----------|----------|--------------------|
| 1   | A     | 632/627 (101%) | 575 (91%) | 57 (9%)  | <b>9</b> <b>32</b> |
| 1   | B     | 630/627 (100%) | 574 (91%) | 56 (9%)  | <b>9</b> <b>33</b> |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | C     | 626/627 (100%)   | 569 (91%)  | 57 (9%)  | 9           | 32 |
| 1   | D     | 632/627 (101%)   | 584 (92%)  | 48 (8%)  | 13          | 40 |
| 1   | E     | 630/627 (100%)   | 579 (92%)  | 51 (8%)  | 11          | 37 |
| 1   | F     | 630/627 (100%)   | 573 (91%)  | 57 (9%)  | 9           | 32 |
| All | All   | 3780/3762 (100%) | 3454 (91%) | 326 (9%) | 10          | 35 |

All (326) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | ARG  |
| 1   | A     | 30  | LEU  |
| 1   | A     | 49  | ARG  |
| 1   | A     | 60  | LEU  |
| 1   | A     | 69  | ARG  |
| 1   | A     | 89  | GLU  |
| 1   | A     | 91  | SER  |
| 1   | A     | 111 | ASP  |
| 1   | A     | 116 | LEU  |
| 1   | A     | 117 | PHE  |
| 1   | A     | 163 | ARG  |
| 1   | A     | 173 | ARG  |
| 1   | A     | 181 | CYS  |
| 1   | A     | 187 | SER  |
| 1   | A     | 188 | TYR  |
| 1   | A     | 193 | SER  |
| 1   | A     | 196 | GLN  |
| 1   | A     | 221 | ILE  |
| 1   | A     | 224 | ILE  |
| 1   | A     | 228 | CYS  |
| 1   | A     | 250 | PHE  |
| 1   | A     | 284 | LEU  |
| 1   | A     | 300 | LEU  |
| 1   | A     | 306 | MSE  |
| 1   | A     | 317 | PHE  |
| 1   | A     | 320 | SER  |
| 1   | A     | 328 | THR  |
| 1   | A     | 347 | GLU  |
| 1   | A     | 357 | LEU  |
| 1   | A     | 375 | ASP  |
| 1   | A     | 399 | ASN  |
| 1   | A     | 438 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 455        | LEU         |
| 1          | A            | 482        | LEU         |
| 1          | A            | 500        | LEU         |
| 1          | A            | 502        | SER         |
| 1          | A            | 516        | ASP         |
| 1          | A            | 523        | GLU         |
| 1          | A            | 529        | TYR         |
| 1          | A            | 537        | HIS         |
| 1          | A            | 547        | ASP         |
| 1          | A            | 587        | TYR         |
| 1          | A            | 615        | LEU         |
| 1          | A            | 627        | ARG         |
| 1          | A            | 640        | SER         |
| 1          | A            | 648        | ASP         |
| 1          | A            | 663        | GLU         |
| 1          | A            | 668        | SER         |
| 1          | A            | 708        | ASN         |
| 1          | A            | 718        | ASN         |
| 1          | A            | 719        | GLU         |
| 1          | A            | 735        | ASN         |
| 1          | A            | 736        | PHE         |
| 1          | A            | 738        | VAL         |
| 1          | A            | 755        | PHE         |
| 1          | A            | 756        | LEU         |
| 1          | A            | 771        | MSE         |
| 1          | B            | 7          | HIS         |
| 1          | B            | 11         | ILE         |
| 1          | B            | 33         | TYR         |
| 1          | B            | 86         | PHE         |
| 1          | B            | 102        | ILE         |
| 1          | B            | 112        | CYS         |
| 1          | B            | 117        | PHE         |
| 1          | B            | 134        | CYS         |
| 1          | B            | 162        | CYS         |
| 1          | B            | 177        | GLU         |
| 1          | B            | 181        | CYS         |
| 1          | B            | 193        | SER         |
| 1          | B            | 221        | ILE         |
| 1          | B            | 224        | ILE         |
| 1          | B            | 225        | HIS         |
| 1          | B            | 228        | CYS         |
| 1          | B            | 241        | ARG         |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 250        | PHE         |
| 1          | B            | 256        | ASP         |
| 1          | B            | 278        | ARG         |
| 1          | B            | 282        | ILE         |
| 1          | B            | 309        | TYR         |
| 1          | B            | 317        | PHE         |
| 1          | B            | 320        | SER         |
| 1          | B            | 328        | THR         |
| 1          | B            | 337        | MSE         |
| 1          | B            | 369        | SER         |
| 1          | B            | 375        | ASP         |
| 1          | B            | 411        | PHE         |
| 1          | B            | 428        | THR         |
| 1          | B            | 438        | ARG         |
| 1          | B            | 439        | GLU         |
| 1          | B            | 444        | PHE         |
| 1          | B            | 445        | ARG         |
| 1          | B            | 471        | MSE         |
| 1          | B            | 482        | LEU         |
| 1          | B            | 488        | TYR         |
| 1          | B            | 490        | HIS         |
| 1          | B            | 500        | LEU         |
| 1          | B            | 516        | ASP         |
| 1          | B            | 527        | LEU         |
| 1          | B            | 540        | TYR         |
| 1          | B            | 547        | ASP         |
| 1          | B            | 587        | TYR         |
| 1          | B            | 592        | PHE         |
| 1          | B            | 653        | VAL         |
| 1          | B            | 663        | GLU         |
| 1          | B            | 699        | GLU         |
| 1          | B            | 704        | PHE         |
| 1          | B            | 718        | ASN         |
| 1          | B            | 736        | PHE         |
| 1          | B            | 738        | VAL         |
| 1          | B            | 747        | ASN         |
| 1          | B            | 755        | PHE         |
| 1          | B            | 760        | TYR         |
| 1          | B            | 771        | MSE         |
| 1          | C            | 33         | TYR         |
| 1          | C            | 61         | TYR         |
| 1          | C            | 89         | GLU         |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | C            | 117        | PHE         |
| 1          | C            | 120        | THR         |
| 1          | C            | 129        | ILE         |
| 1          | C            | 142        | GLU         |
| 1          | C            | 148        | ARG         |
| 1          | C            | 164        | SER         |
| 1          | C            | 172        | ARG         |
| 1          | C            | 173        | ARG         |
| 1          | C            | 181        | CYS         |
| 1          | C            | 193        | SER         |
| 1          | C            | 196        | GLN         |
| 1          | C            | 225        | HIS         |
| 1          | C            | 233        | GLU         |
| 1          | C            | 257        | ILE         |
| 1          | C            | 258        | GLU         |
| 1          | C            | 261        | LYS         |
| 1          | C            | 267        | SER         |
| 1          | C            | 274        | LEU         |
| 1          | C            | 278        | ARG         |
| 1          | C            | 284        | LEU         |
| 1          | C            | 292        | LEU         |
| 1          | C            | 306        | MSE         |
| 1          | C            | 313        | HIS         |
| 1          | C            | 317        | PHE         |
| 1          | C            | 337        | MSE         |
| 1          | C            | 357        | LEU         |
| 1          | C            | 370        | VAL         |
| 1          | C            | 375        | ASP         |
| 1          | C            | 382        | ARG         |
| 1          | C            | 403        | VAL         |
| 1          | C            | 427        | ASN         |
| 1          | C            | 488        | TYR         |
| 1          | C            | 502        | SER         |
| 1          | C            | 516        | ASP         |
| 1          | C            | 523        | GLU         |
| 1          | C            | 541        | TYR         |
| 1          | C            | 543        | LEU         |
| 1          | C            | 548        | LEU         |
| 1          | C            | 587        | TYR         |
| 1          | C            | 605        | THR         |
| 1          | C            | 616        | ASP         |
| 1          | C            | 624        | VAL         |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | C            | 648        | ASP         |
| 1          | C            | 663        | GLU         |
| 1          | C            | 693        | PHE         |
| 1          | C            | 718        | ASN         |
| 1          | C            | 724        | MSE         |
| 1          | C            | 726        | ARG         |
| 1          | C            | 736        | PHE         |
| 1          | C            | 738        | VAL         |
| 1          | C            | 744        | ARG         |
| 1          | C            | 756        | LEU         |
| 1          | C            | 760        | TYR         |
| 1          | C            | 766        | THR         |
| 1          | D            | 7          | HIS         |
| 1          | D            | 60         | LEU         |
| 1          | D            | 112        | CYS         |
| 1          | D            | 113        | LEU         |
| 1          | D            | 117        | PHE         |
| 1          | D            | 164        | SER         |
| 1          | D            | 181        | CYS         |
| 1          | D            | 188        | TYR         |
| 1          | D            | 201        | ASP         |
| 1          | D            | 221        | ILE         |
| 1          | D            | 242        | ARG         |
| 1          | D            | 250        | PHE         |
| 1          | D            | 262        | SER         |
| 1          | D            | 267        | SER         |
| 1          | D            | 270        | GLU         |
| 1          | D            | 295        | ASN         |
| 1          | D            | 306        | MSE         |
| 1          | D            | 313        | HIS         |
| 1          | D            | 317        | PHE         |
| 1          | D            | 367        | ASP         |
| 1          | D            | 375        | ASP         |
| 1          | D            | 382        | ARG         |
| 1          | D            | 399        | ASN         |
| 1          | D            | 403        | VAL         |
| 1          | D            | 423        | GLN         |
| 1          | D            | 427        | ASN         |
| 1          | D            | 437        | MSE         |
| 1          | D            | 473        | MSE         |
| 1          | D            | 475        | ASN         |
| 1          | D            | 494        | VAL         |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | D            | 541        | TYR         |
| 1          | D            | 543        | LEU         |
| 1          | D            | 551        | TYR         |
| 1          | D            | 587        | TYR         |
| 1          | D            | 605        | THR         |
| 1          | D            | 653        | VAL         |
| 1          | D            | 693        | PHE         |
| 1          | D            | 708        | ASN         |
| 1          | D            | 718        | ASN         |
| 1          | D            | 719        | GLU         |
| 1          | D            | 724        | MSE         |
| 1          | D            | 736        | PHE         |
| 1          | D            | 737        | HIS         |
| 1          | D            | 738        | VAL         |
| 1          | D            | 755        | PHE         |
| 1          | D            | 760        | TYR         |
| 1          | D            | 766        | THR         |
| 1          | D            | 771        | MSE         |
| 1          | E            | 33         | TYR         |
| 1          | E            | 62         | LYS         |
| 1          | E            | 67         | LEU         |
| 1          | E            | 75         | LYS         |
| 1          | E            | 84         | ASP         |
| 1          | E            | 110        | ASP         |
| 1          | E            | 112        | CYS         |
| 1          | E            | 117        | PHE         |
| 1          | E            | 128        | PHE         |
| 1          | E            | 147        | ASP         |
| 1          | E            | 172        | ARG         |
| 1          | E            | 181        | CYS         |
| 1          | E            | 196        | GLN         |
| 1          | E            | 224        | ILE         |
| 1          | E            | 225        | HIS         |
| 1          | E            | 241        | ARG         |
| 1          | E            | 259        | THR         |
| 1          | E            | 267        | SER         |
| 1          | E            | 278        | ARG         |
| 1          | E            | 283        | THR         |
| 1          | E            | 301        | HIS         |
| 1          | E            | 309        | TYR         |
| 1          | E            | 313        | HIS         |
| 1          | E            | 317        | PHE         |

*Continued on next page...*



*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | E            | 328        | THR         |
| 1          | E            | 342        | GLU         |
| 1          | E            | 375        | ASP         |
| 1          | E            | 403        | VAL         |
| 1          | E            | 423        | GLN         |
| 1          | E            | 427        | ASN         |
| 1          | E            | 444        | PHE         |
| 1          | E            | 500        | LEU         |
| 1          | E            | 525        | LEU         |
| 1          | E            | 541        | TYR         |
| 1          | E            | 587        | TYR         |
| 1          | E            | 596        | LEU         |
| 1          | E            | 605        | THR         |
| 1          | E            | 616        | ASP         |
| 1          | E            | 630        | TYR         |
| 1          | E            | 643        | PHE         |
| 1          | E            | 663        | GLU         |
| 1          | E            | 668        | SER         |
| 1          | E            | 686        | HIS         |
| 1          | E            | 693        | PHE         |
| 1          | E            | 708        | ASN         |
| 1          | E            | 718        | ASN         |
| 1          | E            | 736        | PHE         |
| 1          | E            | 738        | VAL         |
| 1          | E            | 747        | ASN         |
| 1          | E            | 755        | PHE         |
| 1          | E            | 760        | TYR         |
| 1          | F            | 22         | TYR         |
| 1          | F            | 84         | ASP         |
| 1          | F            | 113        | LEU         |
| 1          | F            | 116        | LEU         |
| 1          | F            | 117        | PHE         |
| 1          | F            | 147        | ASP         |
| 1          | F            | 175        | HIS         |
| 1          | F            | 181        | CYS         |
| 1          | F            | 203        | LEU         |
| 1          | F            | 225        | HIS         |
| 1          | F            | 228        | CYS         |
| 1          | F            | 233        | GLU         |
| 1          | F            | 238        | GLU         |
| 1          | F            | 250        | PHE         |
| 1          | F            | 262        | SER         |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | F            | 284        | LEU         |
| 1          | F            | 301        | HIS         |
| 1          | F            | 312        | THR         |
| 1          | F            | 317        | PHE         |
| 1          | F            | 328        | THR         |
| 1          | F            | 342        | GLU         |
| 1          | F            | 369        | SER         |
| 1          | F            | 384        | SER         |
| 1          | F            | 403        | VAL         |
| 1          | F            | 423        | GLN         |
| 1          | F            | 427        | ASN         |
| 1          | F            | 459        | ASP         |
| 1          | F            | 473        | MSE         |
| 1          | F            | 487        | HIS         |
| 1          | F            | 490        | HIS         |
| 1          | F            | 533        | GLU         |
| 1          | F            | 537        | HIS         |
| 1          | F            | 541        | TYR         |
| 1          | F            | 554        | LEU         |
| 1          | F            | 587        | TYR         |
| 1          | F            | 593        | ASN         |
| 1          | F            | 596        | LEU         |
| 1          | F            | 599        | LEU         |
| 1          | F            | 605        | THR         |
| 1          | F            | 627        | ARG         |
| 1          | F            | 628        | ARG         |
| 1          | F            | 640        | SER         |
| 1          | F            | 643        | PHE         |
| 1          | F            | 653        | VAL         |
| 1          | F            | 663        | GLU         |
| 1          | F            | 686        | HIS         |
| 1          | F            | 695        | HIS         |
| 1          | F            | 704        | PHE         |
| 1          | F            | 708        | ASN         |
| 1          | F            | 719        | GLU         |
| 1          | F            | 736        | PHE         |
| 1          | F            | 738        | VAL         |
| 1          | F            | 750        | ASN         |
| 1          | F            | 755        | PHE         |
| 1          | F            | 760        | TYR         |
| 1          | F            | 766        | THR         |
| 1          | F            | 771        | MSE         |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 26  | HIS  |
| 1   | A     | 121 | ASN  |
| 1   | A     | 171 | ASN  |
| 1   | A     | 196 | GLN  |
| 1   | A     | 247 | GLN  |
| 1   | A     | 295 | ASN  |
| 1   | A     | 331 | ASN  |
| 1   | A     | 427 | ASN  |
| 1   | A     | 452 | ASN  |
| 1   | A     | 475 | ASN  |
| 1   | A     | 485 | GLN  |
| 1   | A     | 575 | ASN  |
| 1   | A     | 593 | ASN  |
| 1   | A     | 718 | ASN  |
| 1   | A     | 737 | HIS  |
| 1   | A     | 747 | ASN  |
| 1   | A     | 750 | ASN  |
| 1   | B     | 5   | HIS  |
| 1   | B     | 13  | GLN  |
| 1   | B     | 36  | ASN  |
| 1   | B     | 121 | ASN  |
| 1   | B     | 171 | ASN  |
| 1   | B     | 247 | GLN  |
| 1   | B     | 295 | ASN  |
| 1   | B     | 318 | HIS  |
| 1   | B     | 331 | ASN  |
| 1   | B     | 399 | ASN  |
| 1   | B     | 427 | ASN  |
| 1   | B     | 475 | ASN  |
| 1   | B     | 483 | GLN  |
| 1   | B     | 485 | GLN  |
| 1   | B     | 490 | HIS  |
| 1   | B     | 575 | ASN  |
| 1   | B     | 593 | ASN  |
| 1   | B     | 623 | ASN  |
| 1   | B     | 667 | GLN  |
| 1   | B     | 695 | HIS  |
| 1   | B     | 735 | ASN  |
| 1   | B     | 747 | ASN  |
| 1   | B     | 750 | ASN  |
| 1   | C     | 9   | GLN  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | C            | 121        | ASN         |
| 1          | C            | 133        | ASN         |
| 1          | C            | 171        | ASN         |
| 1          | C            | 247        | GLN         |
| 1          | C            | 295        | ASN         |
| 1          | C            | 331        | ASN         |
| 1          | C            | 399        | ASN         |
| 1          | C            | 409        | ASN         |
| 1          | C            | 427        | ASN         |
| 1          | C            | 465        | ASN         |
| 1          | C            | 475        | ASN         |
| 1          | C            | 486        | HIS         |
| 1          | C            | 518        | ASN         |
| 1          | C            | 575        | ASN         |
| 1          | C            | 718        | ASN         |
| 1          | C            | 750        | ASN         |
| 1          | D            | 5          | HIS         |
| 1          | D            | 9          | GLN         |
| 1          | D            | 26         | HIS         |
| 1          | D            | 28         | HIS         |
| 1          | D            | 121        | ASN         |
| 1          | D            | 133        | ASN         |
| 1          | D            | 171        | ASN         |
| 1          | D            | 295        | ASN         |
| 1          | D            | 331        | ASN         |
| 1          | D            | 409        | ASN         |
| 1          | D            | 427        | ASN         |
| 1          | D            | 452        | ASN         |
| 1          | D            | 475        | ASN         |
| 1          | D            | 483        | GLN         |
| 1          | D            | 485        | GLN         |
| 1          | D            | 575        | ASN         |
| 1          | D            | 593        | ASN         |
| 1          | D            | 597        | ASN         |
| 1          | D            | 604        | ASN         |
| 1          | D            | 708        | ASN         |
| 1          | D            | 718        | ASN         |
| 1          | D            | 735        | ASN         |
| 1          | D            | 747        | ASN         |
| 1          | D            | 750        | ASN         |
| 1          | E            | 5          | HIS         |
| 1          | E            | 7          | HIS         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 13  | GLN  |
| 1   | E     | 36  | ASN  |
| 1   | E     | 121 | ASN  |
| 1   | E     | 133 | ASN  |
| 1   | E     | 171 | ASN  |
| 1   | E     | 196 | GLN  |
| 1   | E     | 295 | ASN  |
| 1   | E     | 301 | HIS  |
| 1   | E     | 331 | ASN  |
| 1   | E     | 364 | ASN  |
| 1   | E     | 427 | ASN  |
| 1   | E     | 452 | ASN  |
| 1   | E     | 475 | ASN  |
| 1   | E     | 485 | GLN  |
| 1   | E     | 575 | ASN  |
| 1   | E     | 593 | ASN  |
| 1   | E     | 604 | ASN  |
| 1   | E     | 686 | HIS  |
| 1   | E     | 718 | ASN  |
| 1   | E     | 747 | ASN  |
| 1   | E     | 750 | ASN  |
| 1   | E     | 753 | GLN  |
| 1   | F     | 7   | HIS  |
| 1   | F     | 171 | ASN  |
| 1   | F     | 295 | ASN  |
| 1   | F     | 301 | HIS  |
| 1   | F     | 331 | ASN  |
| 1   | F     | 341 | ASN  |
| 1   | F     | 427 | ASN  |
| 1   | F     | 452 | ASN  |
| 1   | F     | 465 | ASN  |
| 1   | F     | 475 | ASN  |
| 1   | F     | 593 | ASN  |
| 1   | F     | 604 | ASN  |
| 1   | F     | 686 | HIS  |
| 1   | F     | 708 | ASN  |
| 1   | F     | 750 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are 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     | 748/772 (96%)   | -0.03  | 14 (1%) 66 58  | 97, 155, 228, 284     | 0     |
| 1   | B     | 744/772 (96%)   | 0.20   | 38 (5%) 28 24  | 115, 179, 293, 361    | 0     |
| 1   | C     | 739/772 (95%)   | -0.02  | 12 (1%) 72 62  | 118, 171, 229, 257    | 0     |
| 1   | D     | 747/772 (96%)   | 0.12   | 27 (3%) 42 35  | 125, 189, 267, 339    | 0     |
| 1   | E     | 744/772 (96%)   | 0.12   | 34 (4%) 32 27  | 110, 183, 285, 327    | 0     |
| 1   | F     | 744/772 (96%)   | 0.19   | 30 (4%) 38 31  | 138, 191, 298, 348    | 0     |
| All | All   | 4466/4632 (96%) | 0.10   | 155 (3%) 44 35 | 97, 179, 272, 361     | 0     |

All (155) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 70  | ILE  | 6.1  |
| 1   | E     | 51  | GLU  | 5.7  |
| 1   | D     | 81  | GLN  | 5.6  |
| 1   | B     | 46  | VAL  | 5.2  |
| 1   | E     | 198 | ILE  | 5.0  |
| 1   | E     | 46  | VAL  | 4.9  |
| 1   | A     | 586 | LYS  | 4.8  |
| 1   | E     | 199 | TYR  | 4.8  |
| 1   | C     | 99  | ASP  | 4.8  |
| 1   | B     | 3   | ALA  | 4.7  |
| 1   | D     | 91  | SER  | 4.4  |
| 1   | B     | 31  | ARG  | 4.4  |
| 1   | A     | 99  | ASP  | 4.3  |
| 1   | F     | 35  | LYS  | 4.3  |
| 1   | F     | 70  | ILE  | 4.2  |
| 1   | F     | 18  | ARG  | 4.1  |
| 1   | E     | 49  | ARG  | 4.0  |
| 1   | B     | 47  | GLU  | 4.0  |
| 1   | B     | 89  | GLU  | 4.0  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | B            | 51         | GLU         | 3.9         |
| 1          | D            | 82         | GLY         | 3.9         |
| 1          | B            | 80         | PRO         | 3.8         |
| 1          | F            | 175        | HIS         | 3.8         |
| 1          | F            | 400        | GLY         | 3.7         |
| 1          | F            | 17         | PHE         | 3.6         |
| 1          | B            | 87         | TYR         | 3.5         |
| 1          | B            | 2          | LYS         | 3.5         |
| 1          | B            | 62         | LYS         | 3.4         |
| 1          | B            | 88         | ILE         | 3.4         |
| 1          | B            | 81         | GLN         | 3.4         |
| 1          | F            | 19         | PRO         | 3.3         |
| 1          | F            | 199        | TYR         | 3.3         |
| 1          | E            | 80         | PRO         | 3.2         |
| 1          | B            | 4          | TYR         | 3.2         |
| 1          | B            | 45         | VAL         | 3.2         |
| 1          | B            | 32         | GLY         | 3.2         |
| 1          | E            | 75         | LYS         | 3.2         |
| 1          | D            | 49         | ARG         | 3.2         |
| 1          | F            | 255        | LYS         | 3.2         |
| 1          | F            | 62         | LYS         | 3.1         |
| 1          | E            | 3          | ALA         | 3.1         |
| 1          | E            | 47         | GLU         | 3.1         |
| 1          | F            | 78         | ILE         | 3.1         |
| 1          | A            | 78         | ILE         | 3.1         |
| 1          | E            | 85         | ARG         | 3.1         |
| 1          | B            | 79         | PRO         | 3.0         |
| 1          | D            | 586        | LYS         | 3.0         |
| 1          | B            | 60         | LEU         | 3.0         |
| 1          | B            | 6          | ILE         | 3.0         |
| 1          | E            | 81         | GLN         | 3.0         |
| 1          | D            | 198        | ILE         | 2.9         |
| 1          | C            | 91         | SER         | 2.9         |
| 1          | D            | 50         | GLU         | 2.9         |
| 1          | B            | 199        | TYR         | 2.9         |
| 1          | B            | 48         | GLY         | 2.8         |
| 1          | F            | 81         | GLN         | 2.8         |
| 1          | E            | 89         | GLU         | 2.8         |
| 1          | F            | 51         | GLU         | 2.8         |
| 1          | E            | 82         | GLY         | 2.8         |
| 1          | B            | 35         | LYS         | 2.7         |
| 1          | B            | 70         | ILE         | 2.7         |

*Continued on next page...*



*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | C            | 586        | LYS         | 2.7         |
| 1          | D            | 547        | ASP         | 2.7         |
| 1          | B            | 61         | TYR         | 2.7         |
| 1          | E            | 71         | ASP         | 2.7         |
| 1          | E            | 73         | ILE         | 2.6         |
| 1          | A            | 70         | ILE         | 2.6         |
| 1          | E            | 396        | PHE         | 2.6         |
| 1          | F            | 73         | ILE         | 2.6         |
| 1          | F            | 90         | LYS         | 2.6         |
| 1          | E            | 48         | GLY         | 2.6         |
| 1          | E            | 4          | TYR         | 2.6         |
| 1          | F            | 75         | LYS         | 2.6         |
| 1          | D            | 75         | LYS         | 2.6         |
| 1          | B            | 78         | ILE         | 2.6         |
| 1          | D            | 80         | PRO         | 2.6         |
| 1          | E            | 56         | PHE         | 2.6         |
| 1          | B            | 59         | ASP         | 2.5         |
| 1          | B            | 75         | LYS         | 2.5         |
| 1          | E            | 53         | ILE         | 2.5         |
| 1          | C            | 70         | ILE         | 2.5         |
| 1          | F            | 254        | ALA         | 2.5         |
| 1          | B            | 179        | THR         | 2.5         |
| 1          | F            | 49         | ARG         | 2.5         |
| 1          | B            | 17         | PHE         | 2.5         |
| 1          | E            | 31         | ARG         | 2.5         |
| 1          | E            | 24         | ILE         | 2.5         |
| 1          | B            | 44         | ILE         | 2.5         |
| 1          | F            | 296        | LEU         | 2.4         |
| 1          | D            | 732        | ASN         | 2.4         |
| 1          | B            | 36         | ASN         | 2.4         |
| 1          | D            | 53         | ILE         | 2.4         |
| 1          | F            | 605        | THR         | 2.4         |
| 1          | E            | 83         | PHE         | 2.4         |
| 1          | F            | 198        | ILE         | 2.4         |
| 1          | D            | 400        | GLY         | 2.4         |
| 1          | D            | 70         | ILE         | 2.4         |
| 1          | E            | 17         | PHE         | 2.4         |
| 1          | A            | 5          | HIS         | 2.4         |
| 1          | F            | 547        | ASP         | 2.4         |
| 1          | F            | 36         | ASN         | 2.4         |
| 1          | E            | 6          | ILE         | 2.4         |
| 1          | B            | 52         | ASP         | 2.4         |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | E            | 542        | PRO         | 2.4         |
| 1          | C            | 604        | ASN         | 2.3         |
| 1          | D            | 99         | ASP         | 2.3         |
| 1          | A            | 547        | ASP         | 2.3         |
| 1          | B            | 83         | PHE         | 2.3         |
| 1          | D            | 76         | LYS         | 2.3         |
| 1          | C            | 376        | GLY         | 2.3         |
| 1          | D            | 542        | PRO         | 2.3         |
| 1          | F            | 46         | VAL         | 2.3         |
| 1          | B            | 169        | PRO         | 2.3         |
| 1          | A            | 75         | LYS         | 2.3         |
| 1          | C            | 732        | ASN         | 2.3         |
| 1          | D            | 3          | ALA         | 2.3         |
| 1          | E            | 52         | ASP         | 2.3         |
| 1          | A            | 77         | GLU         | 2.3         |
| 1          | F            | 27         | GLU         | 2.3         |
| 1          | D            | 78         | ILE         | 2.3         |
| 1          | D            | 733        | GLY         | 2.2         |
| 1          | F            | 26         | HIS         | 2.2         |
| 1          | D            | 30         | LEU         | 2.2         |
| 1          | E            | 87         | TYR         | 2.2         |
| 1          | A            | 73         | ILE         | 2.2         |
| 1          | C            | 75         | LYS         | 2.2         |
| 1          | D            | 737        | HIS         | 2.2         |
| 1          | E            | 5          | HIS         | 2.2         |
| 1          | B            | 82         | GLY         | 2.2         |
| 1          | B            | 178        | PRO         | 2.2         |
| 1          | D            | 395        | PRO         | 2.2         |
| 1          | A            | 3          | ALA         | 2.2         |
| 1          | D            | 83         | PHE         | 2.2         |
| 1          | A            | 199        | TYR         | 2.1         |
| 1          | C            | 87         | TYR         | 2.1         |
| 1          | F            | 4          | TYR         | 2.1         |
| 1          | A            | 46         | VAL         | 2.1         |
| 1          | C            | 603        | ILE         | 2.1         |
| 1          | B            | 34         | VAL         | 2.1         |
| 1          | E            | 25         | ALA         | 2.1         |
| 1          | E            | 30         | LEU         | 2.1         |
| 1          | B            | 77         | GLU         | 2.1         |
| 1          | D            | 728        | VAL         | 2.1         |
| 1          | A            | 52         | ASP         | 2.1         |
| 1          | C            | 330        | ALA         | 2.1         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 732 | ASN  | 2.1  |
| 1   | F     | 85  | ARG  | 2.0  |
| 1   | D     | 51  | GLU  | 2.0  |
| 1   | E     | 586 | LYS  | 2.0  |
| 1   | D     | 361 | LYS  | 2.0  |
| 1   | C     | 47  | GLU  | 2.0  |
| 1   | A     | 605 | THR  | 2.0  |
| 1   | F     | 586 | LYS  | 2.0  |
| 1   | B     | 198 | ILE  | 2.0  |
| 1   | E     | 62  | LYS  | 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 2   | ZN   | B     | 1003 | 1/1   | 0.80 | 0.32 | 180,180,180,180            | 0     |
| 2   | ZN   | D     | 1003 | 1/1   | 0.88 | 0.21 | 202,202,202,202            | 0     |
| 2   | ZN   | F     | 1002 | 1/1   | 0.89 | 0.11 | 213,213,213,213            | 0     |
| 2   | ZN   | F     | 1001 | 1/1   | 0.90 | 0.27 | 187,187,187,187            | 0     |
| 2   | ZN   | E     | 1002 | 1/1   | 0.91 | 0.08 | 175,175,175,175            | 0     |
| 2   | ZN   | A     | 1003 | 1/1   | 0.94 | 0.24 | 178,178,178,178            | 0     |
| 2   | ZN   | D     | 1002 | 1/1   | 0.94 | 0.08 | 149,149,149,149            | 0     |
| 2   | ZN   | C     | 1001 | 1/1   | 0.95 | 0.19 | 143,143,143,143            | 0     |
| 2   | ZN   | C     | 1002 | 1/1   | 0.95 | 0.13 | 147,147,147,147            | 0     |
| 2   | ZN   | C     | 1003 | 1/1   | 0.96 | 0.23 | 156,156,156,156            | 0     |
| 2   | ZN   | E     | 1003 | 1/1   | 0.97 | 0.21 | 183,183,183,183            | 0     |
| 2   | ZN   | B     | 1002 | 1/1   | 0.98 | 0.03 | 187,187,187,187            | 0     |
| 2   | ZN   | E     | 1001 | 1/1   | 0.98 | 0.26 | 152,152,152,152            | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | ZN   | F     | 1003 | 1/1   | 0.98 | 0.25 | 179,179,179,179             | 0     |
| 2   | ZN   | B     | 1001 | 1/1   | 0.98 | 0.22 | 170,170,170,170             | 0     |
| 2   | ZN   | A     | 1001 | 1/1   | 0.98 | 0.28 | 144,144,144,144             | 0     |
| 2   | ZN   | A     | 1002 | 1/1   | 0.99 | 0.12 | 113,113,113,113             | 0     |
| 2   | ZN   | D     | 1001 | 1/1   | 0.99 | 0.25 | 157,157,157,157             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.