



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:51 AM GMT

PDB ID : 2EIV  
Title : Crystal Structure of the arginase from *Thermus thermophilus*  
Authors : Kumarevel, T.S.; Karthe, P.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2007-03-13  
Resolution : 2.91 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

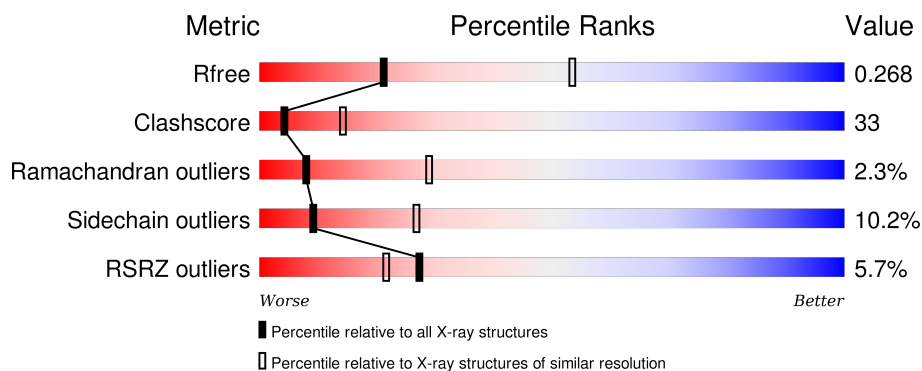
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1643 (2.94-2.90)                                      |
| Clashscore            | 102246                      | 1871 (2.94-2.90)                                      |
| Ramachandran outliers | 100387                      | 1824 (2.94-2.90)                                      |
| Sidechain outliers    | 100360                      | 1826 (2.94-2.90)                                      |
| RSRZ outliers         | 91569                       | 1650 (2.94-2.90)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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     | 291    | <div> <div> <div></div> <div>53%</div> <div>37%</div> <div>6%</div> </div> </div>                 |
| 1   | C     | 291    | <div> <div> <div></div> <div>57%</div> <div>33%</div> <div>6%</div> </div> </div>                 |
| 1   | D     | 291    | <div> <div> <div>3%</div> <div>55%</div> <div>35%</div> <div>6%</div> </div> </div>               |
| 1   | E     | 291    | <div> <div> <div>3%</div> <div>52%</div> <div>36%</div> <div>6%</div> <div>6%</div> </div> </div> |
| 1   | F     | 291    | <div> <div> <div></div> <div>55%</div> <div>33%</div> <div>5%</div> <div>6%</div> </div> </div>   |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain |    |
|-----|-------|--------|------------------|----|
| 1   | G     | 291    |                  | 6% |
| 1   | H     | 291    |                  | 6% |
| 1   | I     | 291    |                  | 6% |
| 1   | J     | 291    |                  | 6% |
| 1   | K     | 291    |                  | 6% |
| 1   | L     | 291    |                  | 6% |
| 1   | M     | 291    |                  | 6% |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 24799 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 Arginase.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |
| 1   | C     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |
| 1   | D     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |
| 1   | E     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |
| 1   | F     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |
| 1   | G     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |
| 1   | H     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |
| 1   | I     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |
| 1   | J     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |
| 1   | K     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |
| 1   | L     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |
| 1   | M     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1300 | 363 | 382 | 7 |         |         |       |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 2   | C     | 12       | Total | O  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |

*Continued on next page...*

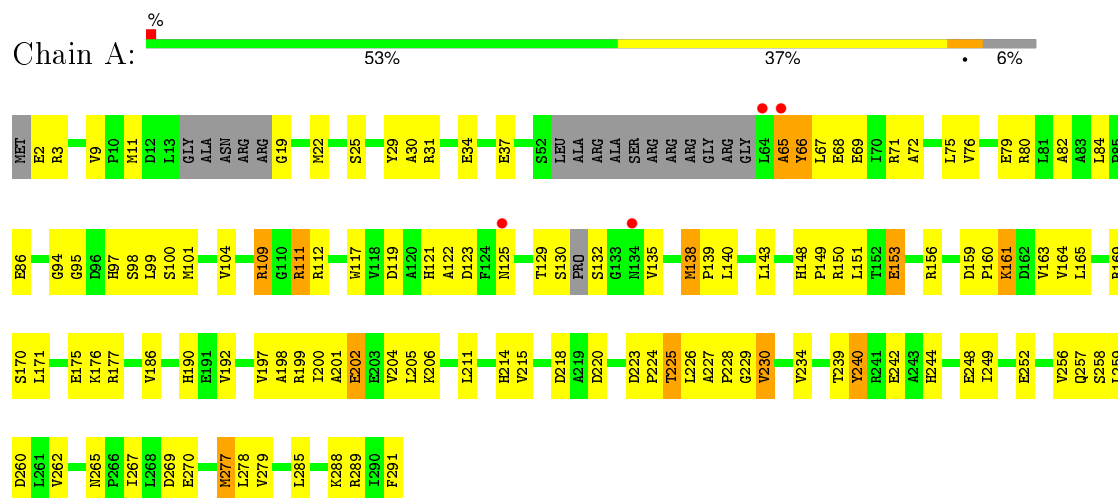
*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 2   | D     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 2   | E     | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 2   | F     | 17       | Total<br>17 | O<br>17 | 0       | 0       |
| 2   | G     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 2   | H     | 19       | Total<br>19 | O<br>19 | 0       | 0       |
| 2   | I     | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 2   | J     | 17       | Total<br>17 | O<br>17 | 0       | 0       |
| 2   | K     | 5        | Total<br>5  | O<br>5  | 0       | 0       |
| 2   | L     | 17       | Total<br>17 | O<br>17 | 0       | 0       |
| 2   | M     | 11       | Total<br>11 | O<br>11 | 0       | 0       |

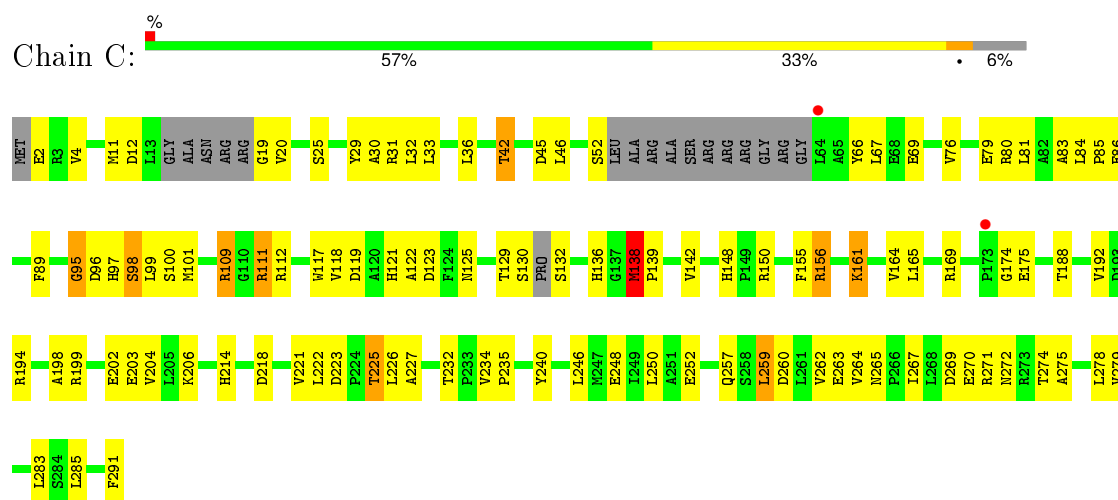
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Arginase

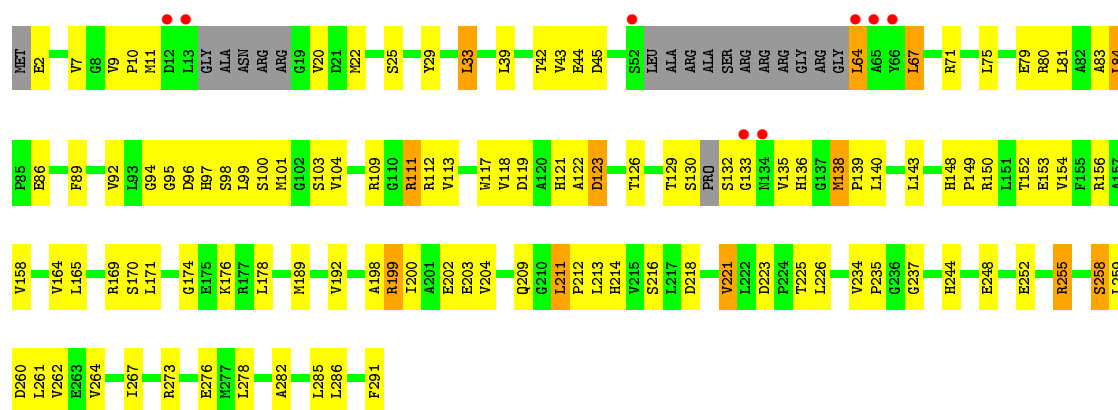


#### • Molecule 1: Arginase

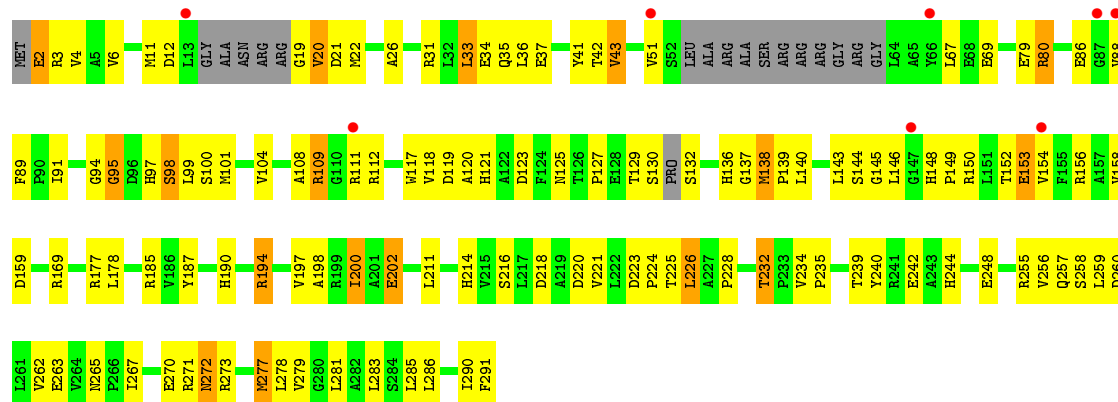


#### • Molecule 1: Arginase

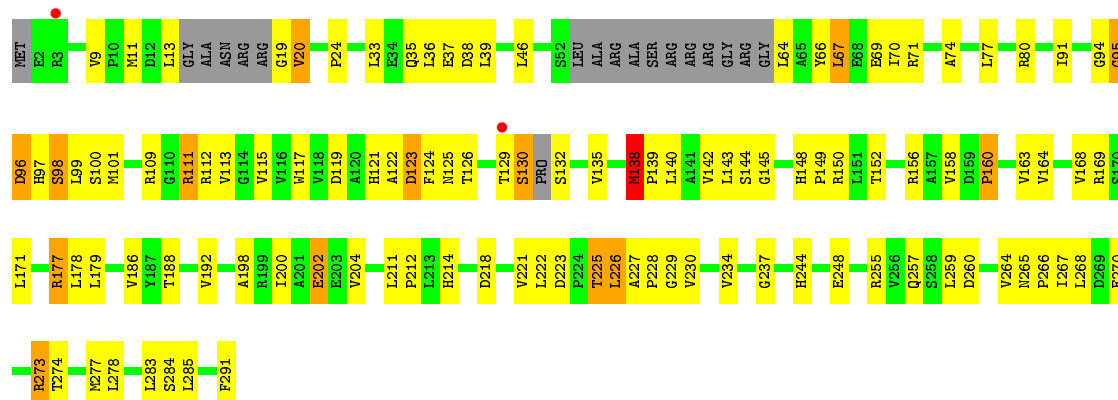




• Molecule 1: Arginase

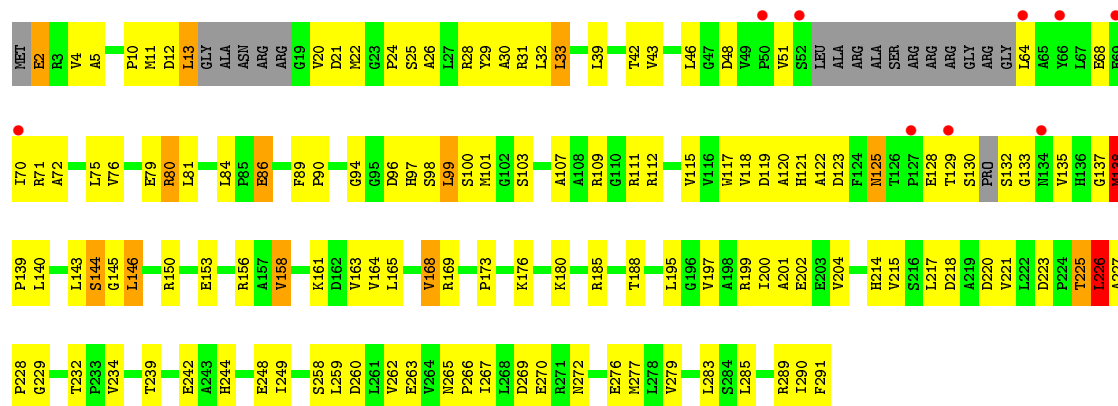


• Molecule 1: Arginase

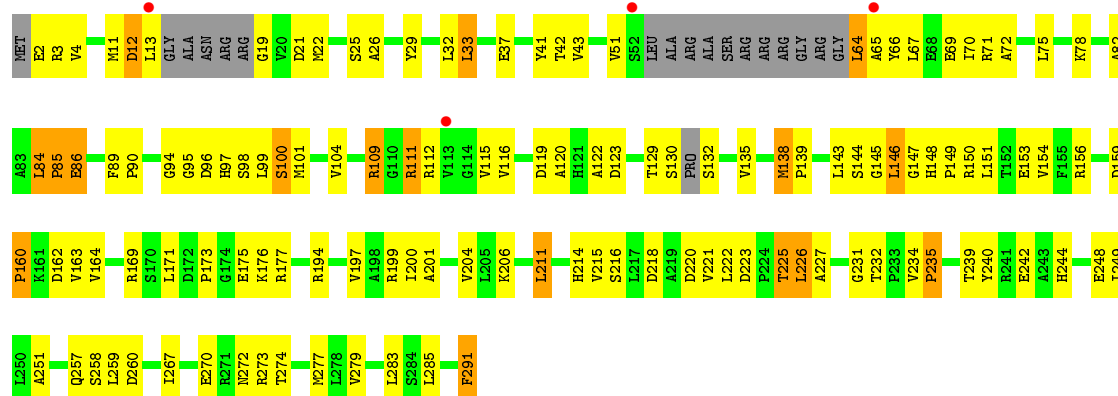


• Molecule 1: Arginase

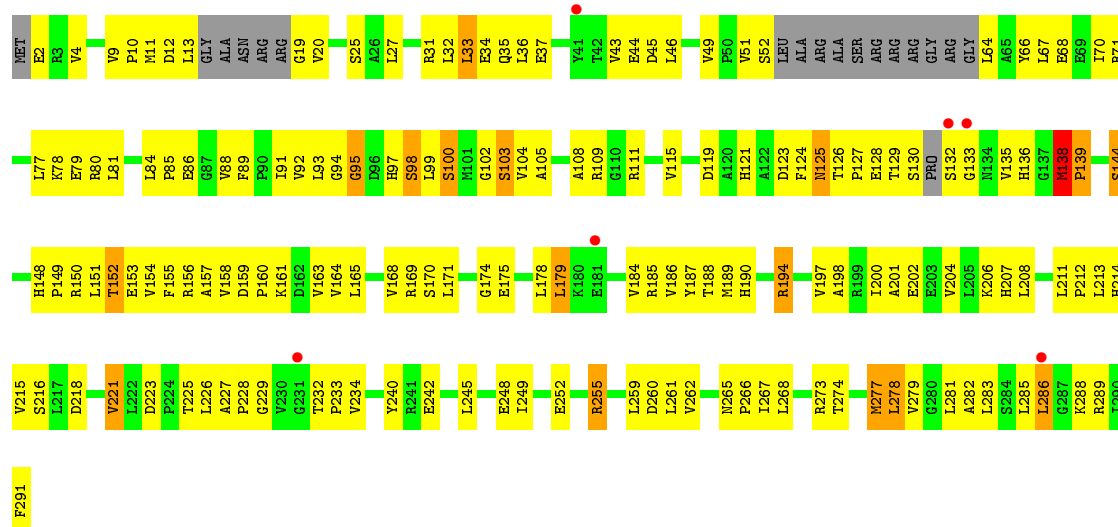




• Molecule 1: Arginase

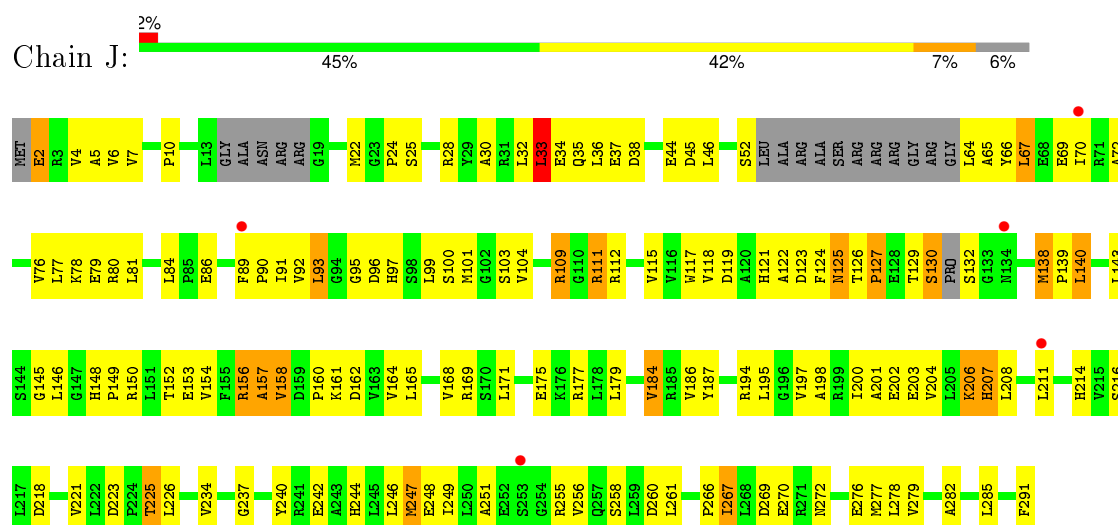


• Molecule 1: Arginase

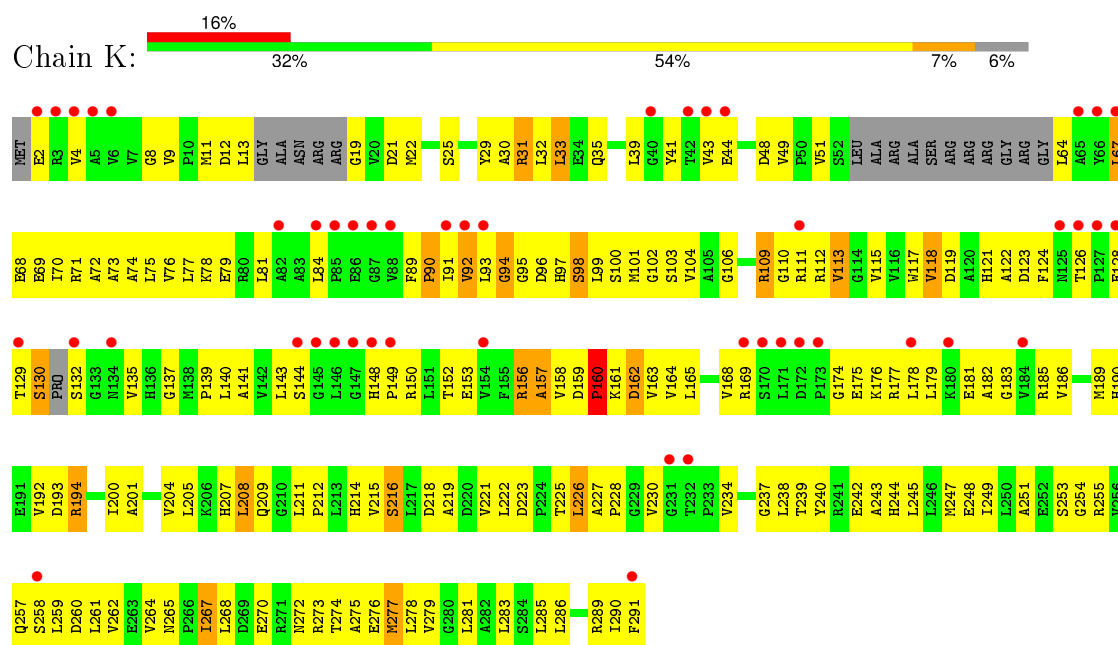


• Molecule 1: Arginase

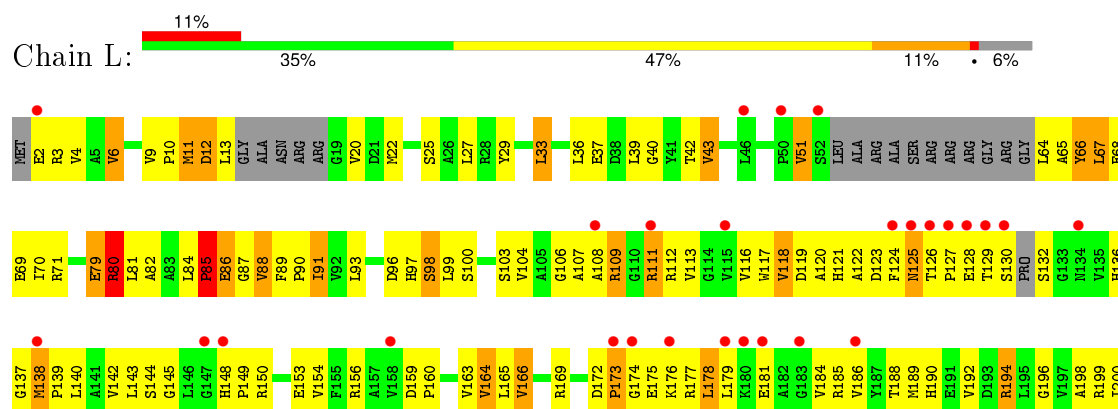


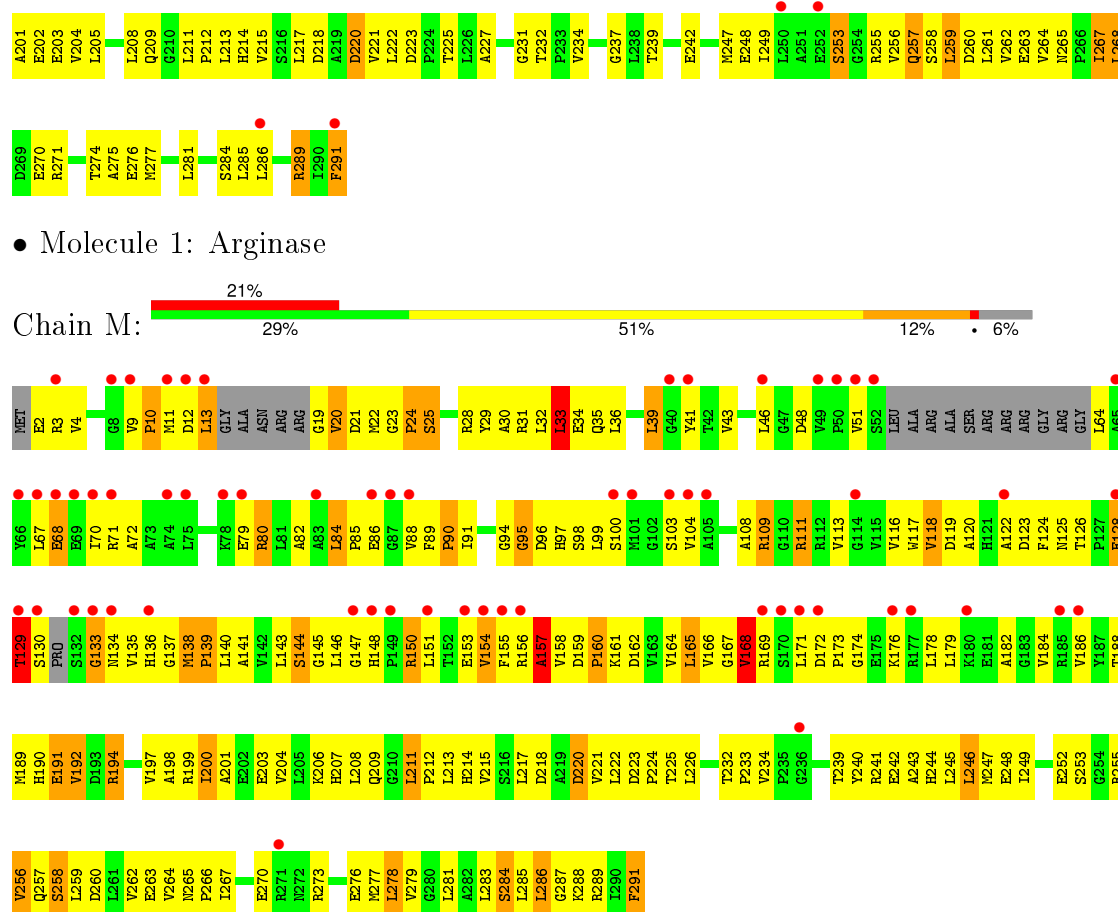


• Molecule 1: Arginase



• Molecule 1: Arginase





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 159.98Å 139.89Å 84.37Å<br>90.00° 90.26° 90.00°              | Depositor        |
| Resolution (Å)  | 20.00 – 2.91<br>39.99 – 2.91                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.9 (20.00-2.91)<br>99.0 (39.99-2.91)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.08  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.14 (at 2.90Å)   | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.232 , 0.269<br>0.231 , 0.268                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4069 reflections (5.05%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 60.3  | Xtriage          |
| Anisotropy  | 0.511   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 67.5   | EDS              |
| Estimated twinning fraction   | 0.019 for -h,-k,l   | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Outliers  | 1 of 80760 reflections (0.001%)                             | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 24799   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 55.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 1   | A     | 0.52         | 0/2083  | 0.83        | 2/2828 (0.1%)   |
| 1   | C     | 0.53         | 0/2083  | 0.81        | 2/2828 (0.1%)   |
| 1   | D     | 0.53         | 0/2083  | 0.82        | 2/2828 (0.1%)   |
| 1   | E     | 0.51         | 0/2083  | 0.80        | 1/2828 (0.0%)   |
| 1   | F     | 0.50         | 0/2083  | 0.81        | 1/2828 (0.0%)   |
| 1   | G     | 0.49         | 0/2083  | 0.83        | 2/2828 (0.1%)   |
| 1   | H     | 0.48         | 0/2083  | 0.83        | 2/2828 (0.1%)   |
| 1   | I     | 0.49         | 0/2083  | 0.83        | 2/2828 (0.1%)   |
| 1   | J     | 0.46         | 0/2083  | 0.80        | 1/2828 (0.0%)   |
| 1   | K     | 0.45         | 0/2083  | 0.83        | 2/2828 (0.1%)   |
| 1   | L     | 0.45         | 0/2083  | 0.83        | 0/2828          |
| 1   | M     | 0.49         | 0/2083  | 0.89        | 5/2828 (0.2%)   |
| All | All   | 0.49         | 0/24996 | 0.83        | 22/33936 (0.1%) |

There are no bond length outliers.

All (22) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | I     | 133 | GLY  | N-CA-C   | 9.38  | 136.55      | 113.10   |
| 1   | J     | 95  | GLY  | N-CA-C   | -8.96 | 90.71       | 113.10   |
| 1   | M     | 157 | ALA  | CB-CA-C  | 8.88  | 123.42      | 110.10   |
| 1   | M     | 95  | GLY  | N-CA-C   | -7.86 | 93.46       | 113.10   |
| 1   | I     | 95  | GLY  | N-CA-C   | -7.57 | 94.17       | 113.10   |
| 1   | M     | 133 | GLY  | N-CA-C   | 7.33  | 131.43      | 113.10   |
| 1   | A     | 95  | GLY  | N-CA-C   | -7.12 | 95.29       | 113.10   |
| 1   | E     | 95  | GLY  | N-CA-C   | -6.53 | 96.79       | 113.10   |
| 1   | F     | 95  | GLY  | N-CA-C   | -6.51 | 96.83       | 113.10   |
| 1   | H     | 95  | GLY  | N-CA-C   | -6.38 | 97.15       | 113.10   |
| 1   | M     | 158 | VAL  | N-CA-CB  | -6.22 | 97.81       | 111.50   |
| 1   | G     | 64  | LEU  | CA-CB-CG | 6.19  | 129.54      | 115.30   |
| 1   | D     | 42  | THR  | N-CA-C   | -5.90 | 95.07       | 111.00   |
| 1   | D     | 133 | GLY  | N-CA-C   | 5.81  | 127.63      | 113.10   |
| 1   | C     | 42  | THR  | N-CA-C   | -5.76 | 95.44       | 111.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 66  | TYR  | N-CA-C   | 5.64  | 126.24      | 111.00   |
| 1   | C     | 95  | GLY  | N-CA-C   | -5.62 | 99.05       | 113.10   |
| 1   | H     | 226 | LEU  | CA-CB-CG | 5.60  | 128.18      | 115.30   |
| 1   | K     | 94  | GLY  | N-CA-C   | 5.47  | 126.78      | 113.10   |
| 1   | K     | 95  | GLY  | N-CA-C   | -5.39 | 99.61       | 113.10   |
| 1   | M     | 165 | LEU  | CA-CB-CG | -5.28 | 103.16      | 115.30   |
| 1   | G     | 226 | LEU  | CA-CB-CG | 5.20  | 127.25      | 115.30   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2052  | 0        | 2101     | 129     | 0            |
| 1   | C     | 2052  | 0        | 2101     | 119     | 0            |
| 1   | D     | 2052  | 0        | 2101     | 127     | 0            |
| 1   | E     | 2052  | 0        | 2101     | 112     | 0            |
| 1   | F     | 2052  | 0        | 2101     | 104     | 0            |
| 1   | G     | 2052  | 0        | 2101     | 111     | 0            |
| 1   | H     | 2052  | 0        | 2101     | 138     | 0            |
| 1   | I     | 2052  | 0        | 2101     | 147     | 0            |
| 1   | J     | 2052  | 0        | 2101     | 151     | 0            |
| 1   | K     | 2052  | 0        | 2101     | 178     | 0            |
| 1   | L     | 2052  | 0        | 2101     | 179     | 0            |
| 1   | M     | 2052  | 0        | 2101     | 234     | 0            |
| 2   | A     | 26    | 0        | 0        | 1       | 0            |
| 2   | C     | 12    | 0        | 0        | 2       | 0            |
| 2   | D     | 9     | 0        | 0        | 2       | 0            |
| 2   | E     | 18    | 0        | 0        | 4       | 0            |
| 2   | F     | 17    | 0        | 0        | 2       | 0            |
| 2   | G     | 10    | 0        | 0        | 2       | 0            |
| 2   | H     | 19    | 0        | 0        | 2       | 0            |
| 2   | I     | 14    | 0        | 0        | 1       | 0            |
| 2   | J     | 17    | 0        | 0        | 3       | 0            |
| 2   | K     | 5     | 0        | 0        | 2       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | L     | 17    | 0        | 0        | 5       | 0            |
| 2   | M     | 11    | 0        | 0        | 6       | 0            |
| All | All   | 24799 | 0        | 25212    | 1655    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1655) 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:111:ARG:NH2  | 1:D:79:GLU:HA    | 1.57                     | 1.19              |
| 1:F:111:ARG:HD3  | 1:F:112:ARG:N    | 1.62                     | 1.14              |
| 1:F:111:ARG:HD3  | 1:F:112:ARG:H    | 0.97                     | 1.11              |
| 1:H:109:ARG:HG2  | 1:H:109:ARG:HH11 | 1.05                     | 1.11              |
| 1:A:79:GLU:HB3   | 1:D:111:ARG:HH22 | 1.16                     | 1.10              |
| 1:J:109:ARG:HH11 | 1:J:109:ARG:HB3  | 1.11                     | 1.10              |
| 1:C:109:ARG:HH11 | 1:C:109:ARG:HG2  | 0.92                     | 1.09              |
| 1:H:111:ARG:HD3  | 1:H:112:ARG:H    | 1.17                     | 1.08              |
| 1:F:130:SER:HG   | 1:F:132:SER:N    | 1.52                     | 1.08              |
| 1:J:130:SER:HG   | 1:J:132:SER:N    | 1.52                     | 1.07              |
| 1:L:111:ARG:HD3  | 1:L:112:ARG:H    | 1.14                     | 1.06              |
| 1:M:138:MET:H    | 1:M:139:PRO:HD2  | 1.17                     | 1.04              |
| 1:M:129:THR:HB   | 1:M:174:GLY:HA3  | 1.38                     | 1.03              |
| 1:G:145:GLY:HA2  | 1:G:156:ARG:HD3  | 1.39                     | 1.01              |
| 1:K:113:VAL:HG12 | 1:K:212:PRO:HG2  | 1.41                     | 1.01              |
| 1:K:130:SER:HG   | 1:K:132:SER:N    | 1.59                     | 0.98              |
| 1:L:109:ARG:HH11 | 1:L:109:ARG:HG2  | 1.26                     | 0.98              |
| 1:H:111:ARG:CD   | 1:H:112:ARG:H    | 1.77                     | 0.97              |
| 1:C:109:ARG:HG2  | 1:C:109:ARG:NH1  | 1.72                     | 0.96              |
| 1:I:130:SER:HG   | 1:I:132:SER:N    | 1.64                     | 0.94              |
| 1:J:72:ALA:O     | 1:J:76:VAL:HG23  | 1.66                     | 0.94              |
| 1:L:138:MET:H    | 1:L:139:PRO:HD2  | 1.32                     | 0.94              |
| 1:M:113:VAL:HA   | 2:M:296:HOH:O    | 1.68                     | 0.93              |
| 1:A:111:ARG:HH21 | 1:D:79:GLU:HA    | 1.13                     | 0.93              |
| 1:M:145:GLY:HA3  | 1:M:156:ARG:HH11 | 1.32                     | 0.93              |
| 1:M:140:LEU:HA   | 1:M:143:LEU:HD12 | 1.50                     | 0.93              |
| 1:M:199:ARG:O    | 1:M:203:GLU:HG3  | 1.69                     | 0.92              |
| 1:C:86:GLU:HG2   | 1:C:109:ARG:HE   | 1.35                     | 0.92              |
| 1:K:111:ARG:HD3  | 1:K:112:ARG:H    | 1.34                     | 0.92              |
| 1:C:271:ARG:NH2  | 1:K:228:PRO:HB2  | 1.84                     | 0.92              |
| 1:H:111:ARG:HE   | 1:H:111:ARG:HA   | 1.34                     | 0.91              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:111:ARG:HD3  | 1:H:112:ARG:N    | 1.85                     | 0.91              |
| 1:M:80:ARG:HG2   | 1:M:80:ARG:HH11  | 1.36                     | 0.91              |
| 1:M:138:MET:N    | 1:M:139:PRO:HD2  | 1.85                     | 0.91              |
| 1:E:138:MET:N    | 1:E:139:PRO:HD2  | 1.86                     | 0.91              |
| 1:G:101:MET:HA   | 1:G:143:LEU:HD21 | 1.53                     | 0.91              |
| 1:K:123:ASP:HB3  | 1:K:139:PRO:HD2  | 1.52                     | 0.90              |
| 1:K:227:ALA:HB1  | 1:K:274:THR:HG23 | 1.53                     | 0.90              |
| 1:H:109:ARG:NH1  | 1:H:109:ARG:HG2  | 1.85                     | 0.90              |
| 1:A:79:GLU:CB    | 1:D:111:ARG:HH22 | 1.85                     | 0.90              |
| 1:H:223:ASP:OD2  | 1:H:225:THR:HB   | 1.72                     | 0.90              |
| 1:J:216:SER:HA   | 1:J:260:ASP:HB2  | 1.51                     | 0.90              |
| 1:G:117:TRP:HB3  | 1:G:165:LEU:HD23 | 1.52                     | 0.89              |
| 1:K:259:LEU:HD22 | 1:K:285:LEU:HD23 | 1.55                     | 0.89              |
| 1:H:4:VAL:HG22   | 1:H:89:PHE:HB3   | 1.53                     | 0.89              |
| 1:A:111:ARG:NH2  | 1:D:79:GLU:CA    | 2.34                     | 0.88              |
| 1:H:111:ARG:HA   | 1:H:111:ARG:NE   | 1.84                     | 0.88              |
| 1:C:83:ALA:C     | 1:H:111:ARG:HH12 | 1.77                     | 0.88              |
| 1:J:109:ARG:NH1  | 1:J:109:ARG:HB3  | 1.89                     | 0.88              |
| 1:E:138:MET:H    | 1:E:139:PRO:HD2  | 1.38                     | 0.88              |
| 1:M:153:GLU:HG3  | 1:M:154:VAL:H    | 1.39                     | 0.88              |
| 1:C:79:GLU:HB2   | 1:H:86:GLU:OE1   | 1.73                     | 0.87              |
| 1:I:197:VAL:HG21 | 1:I:242:GLU:HB3  | 1.57                     | 0.87              |
| 1:L:33:LEU:HD23  | 1:L:43:VAL:HB    | 1.56                     | 0.87              |
| 1:H:197:VAL:HG21 | 1:H:242:GLU:HG2  | 1.55                     | 0.87              |
| 1:D:111:ARG:HE   | 1:D:112:ARG:H    | 1.23                     | 0.87              |
| 1:I:227:ALA:HB1  | 1:I:274:THR:HG23 | 1.56                     | 0.87              |
| 1:K:164:VAL:HG23 | 1:K:208:LEU:HD11 | 1.56                     | 0.86              |
| 1:K:129:THR:O    | 1:K:130:SER:HB2  | 1.75                     | 0.85              |
| 1:J:164:VAL:HG11 | 1:J:204:VAL:HG22 | 1.58                     | 0.85              |
| 1:M:111:ARG:HA   | 1:M:111:ARG:HE   | 1.41                     | 0.85              |
| 1:L:111:ARG:HD3  | 1:L:112:ARG:N    | 1.92                     | 0.85              |
| 1:C:148:HIS:HD2  | 1:C:150:ARG:H    | 1.25                     | 0.85              |
| 1:A:111:ARG:HD3  | 1:A:112:ARG:H    | 1.42                     | 0.85              |
| 1:J:125:ASN:ND2  | 1:J:175:GLU:HG3  | 1.92                     | 0.85              |
| 1:L:223:ASP:HB3  | 1:L:225:THR:HG22 | 1.58                     | 0.85              |
| 1:M:82:ALA:HA    | 1:M:109:ARG:HH12 | 1.42                     | 0.85              |
| 1:C:83:ALA:HB1   | 1:H:111:ARG:CZ   | 2.07                     | 0.84              |
| 1:I:36:LEU:HD21  | 1:I:286:LEU:HD23 | 1.59                     | 0.84              |
| 1:G:125:ASN:O    | 1:G:138:MET:HB3  | 1.78                     | 0.84              |
| 1:A:111:ARG:HH12 | 1:D:83:ALA:HB2   | 1.42                     | 0.84              |
| 1:L:25:SER:O     | 1:L:29:TYR:HD2   | 1.60                     | 0.84              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:197:VAL:HG21 | 1:E:242:GLU:HG2  | 1.58                     | 0.84              |
| 1:F:111:ARG:CD   | 1:F:112:ARG:H    | 1.88                     | 0.83              |
| 1:H:109:ARG:HH11 | 1:H:109:ARG:CG   | 1.91                     | 0.83              |
| 1:H:239:THR:OG1  | 1:H:242:GLU:HB2  | 1.78                     | 0.83              |
| 1:I:4:VAL:HG22   | 1:I:89:PHE:HB3   | 1.60                     | 0.83              |
| 1:J:156:ARG:HH11 | 1:J:156:ARG:HG2  | 1.42                     | 0.83              |
| 1:F:244:HIS:O    | 1:F:248:GLU:HG3  | 1.79                     | 0.83              |
| 1:J:195:LEU:HD12 | 1:J:200:ILE:HD11 | 1.60                     | 0.83              |
| 1:L:4:VAL:HG22   | 1:L:89:PHE:HB3   | 1.58                     | 0.83              |
| 1:F:148:HIS:HD2  | 1:F:150:ARG:H    | 1.27                     | 0.83              |
| 1:J:109:ARG:HH11 | 1:J:109:ARG:CB   | 1.89                     | 0.83              |
| 1:J:66:TYR:O     | 1:J:70:ILE:HD13  | 1.79                     | 0.82              |
| 1:M:226:LEU:HD21 | 1:M:240:TYR:HB2  | 1.59                     | 0.82              |
| 1:H:82:ALA:HA    | 1:H:109:ARG:HH12 | 1.44                     | 0.82              |
| 1:C:83:ALA:O     | 1:H:111:ARG:NH1  | 2.13                     | 0.81              |
| 1:L:138:MET:N    | 1:L:139:PRO:HD2  | 1.95                     | 0.81              |
| 1:K:200:ILE:O    | 1:K:204:VAL:HG23 | 1.79                     | 0.81              |
| 1:L:215:VAL:HG21 | 1:L:285:LEU:HD21 | 1.61                     | 0.81              |
| 1:L:138:MET:H    | 1:L:139:PRO:CD   | 1.92                     | 0.81              |
| 1:I:138:MET:N    | 1:I:139:PRO:HD2  | 1.94                     | 0.81              |
| 1:M:34:GLU:H     | 1:M:34:GLU:CD    | 1.85                     | 0.81              |
| 1:L:138:MET:HA   | 2:L:301:HOH:O    | 1.80                     | 0.81              |
| 1:L:190:HIS:HE1  | 1:L:194:ARG:HE   | 1.27                     | 0.81              |
| 1:A:138:MET:N    | 1:A:139:PRO:HD2  | 1.96                     | 0.81              |
| 1:M:36:LEU:HD21  | 1:M:286:LEU:HD23 | 1.62                     | 0.80              |
| 1:A:79:GLU:HB3   | 1:D:111:ARG:NH2  | 1.96                     | 0.80              |
| 1:F:227:ALA:HB1  | 1:F:274:THR:HG23 | 1.63                     | 0.80              |
| 1:M:13:LEU:HD12  | 1:M:70:ILE:HG12  | 1.61                     | 0.80              |
| 1:L:165:LEU:HD12 | 1:L:186:VAL:CG2  | 2.11                     | 0.80              |
| 1:J:138:MET:N    | 1:J:139:PRO:HD2  | 1.96                     | 0.80              |
| 1:E:119:ASP:HA   | 1:E:218:ASP:HB3  | 1.64                     | 0.80              |
| 1:F:119:ASP:OD2  | 1:F:123:ASP:OD2  | 2.00                     | 0.80              |
| 1:I:67:LEU:C     | 1:I:67:LEU:HD23  | 2.02                     | 0.80              |
| 1:M:113:VAL:HG12 | 1:M:212:PRO:HG2  | 1.61                     | 0.80              |
| 1:E:130:SER:HG   | 1:E:132:SER:N    | 1.80                     | 0.80              |
| 1:E:37:GLU:HG2   | 1:E:43:VAL:HG23  | 1.64                     | 0.79              |
| 1:H:216:SER:HA   | 1:H:260:ASP:HB2  | 1.64                     | 0.79              |
| 1:A:130:SER:HG   | 1:A:132:SER:N    | 1.80                     | 0.79              |
| 1:C:109:ARG:HH11 | 1:C:109:ARG:CG   | 1.85                     | 0.79              |
| 1:G:197:VAL:HG21 | 1:G:242:GLU:HB3  | 1.63                     | 0.79              |
| 1:M:211:LEU:HB3  | 2:M:296:HOH:O    | 1.83                     | 0.78              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:193:ASP:HB3  | 1:M:245:LEU:HD22 | 1.65                     | 0.78              |
| 1:E:153:GLU:HG3  | 1:E:154:VAL:HG13 | 1.65                     | 0.78              |
| 1:M:208:LEU:O    | 1:M:211:LEU:HG   | 1.83                     | 0.78              |
| 1:C:218:ASP:OD2  | 2:C:292:HOH:O    | 1.99                     | 0.78              |
| 1:K:144:SER:HB3  | 1:K:160:PRO:HG3  | 1.66                     | 0.78              |
| 1:F:259:LEU:HD13 | 1:F:285:LEU:HD23 | 1.65                     | 0.78              |
| 1:E:120:ALA:HB2  | 1:E:220:ASP:O    | 1.82                     | 0.78              |
| 1:M:218:ASP:HA   | 1:M:262:VAL:HG23 | 1.65                     | 0.78              |
| 1:A:111:ARG:HD3  | 1:A:112:ARG:N    | 1.98                     | 0.78              |
| 1:H:259:LEU:HD13 | 1:H:285:LEU:HD23 | 1.66                     | 0.78              |
| 1:I:164:VAL:HG22 | 1:I:185:ARG:HB3  | 1.66                     | 0.78              |
| 1:M:12:ASP:HB2   | 1:M:21:ASP:HB3   | 1.66                     | 0.78              |
| 1:G:138:MET:N    | 1:G:139:PRO:HD2  | 1.99                     | 0.77              |
| 1:M:168:VAL:HG12 | 1:M:188:THR:HA   | 1.67                     | 0.77              |
| 1:E:145:GLY:O    | 1:E:146:LEU:HD23 | 1.84                     | 0.77              |
| 1:G:109:ARG:HG2  | 1:G:109:ARG:HH11 | 1.50                     | 0.77              |
| 1:G:12:ASP:O     | 1:G:13:LEU:HD23  | 1.85                     | 0.77              |
| 1:G:272:ASN:O    | 1:G:276:GLU:HG3  | 1.84                     | 0.77              |
| 1:M:109:ARG:HH11 | 1:M:109:ARG:HG2  | 1.49                     | 0.77              |
| 1:C:84:LEU:O     | 1:C:109:ARG:NH2  | 2.19                     | 0.76              |
| 1:C:97:HIS:ND1   | 1:C:123:ASP:OD2  | 2.18                     | 0.76              |
| 1:L:122:ALA:HB3  | 1:L:175:GLU:OE2  | 1.84                     | 0.76              |
| 1:C:164:VAL:HG11 | 1:C:204:VAL:HG22 | 1.66                     | 0.76              |
| 1:K:109:ARG:HB3  | 1:K:109:ARG:HH11 | 1.50                     | 0.76              |
| 1:A:149:PRO:O    | 1:A:153:GLU:HB3  | 1.85                     | 0.76              |
| 1:I:109:ARG:HH11 | 1:I:109:ARG:HG2  | 1.48                     | 0.76              |
| 1:K:19:GLY:HA3   | 1:K:265:ASN:ND2  | 2.01                     | 0.76              |
| 1:M:111:ARG:HA   | 1:M:111:ARG:NE   | 1.99                     | 0.76              |
| 1:K:12:ASP:HB2   | 1:K:21:ASP:HB3   | 1.68                     | 0.76              |
| 1:M:146:LEU:HD13 | 1:M:178:LEU:HD22 | 1.67                     | 0.76              |
| 1:F:101:MET:HA   | 1:F:143:LEU:HD21 | 1.67                     | 0.75              |
| 1:C:19:GLY:N     | 1:C:265:ASN:HD21 | 1.84                     | 0.75              |
| 1:G:4:VAL:HG22   | 1:G:89:PHE:HB3   | 1.68                     | 0.75              |
| 1:M:138:MET:H    | 1:M:139:PRO:CD   | 1.97                     | 0.75              |
| 1:K:165:LEU:HD12 | 1:K:186:VAL:HG22 | 1.69                     | 0.75              |
| 1:J:100:SER:HA   | 1:J:103:SER:OG   | 1.86                     | 0.75              |
| 1:D:11:MET:CE    | 1:D:98:SER:HB2   | 2.15                     | 0.75              |
| 1:J:168:VAL:HG11 | 1:J:171:LEU:HD21 | 1.69                     | 0.75              |
| 1:M:145:GLY:HA2  | 1:M:156:ARG:CG   | 2.17                     | 0.75              |
| 1:H:11:MET:CE    | 1:H:98:SER:HB2   | 2.17                     | 0.75              |
| 1:M:168:VAL:HG21 | 1:M:171:LEU:HD21 | 1.69                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:115:VAL:HG23 | 1:G:158:VAL:HG21 | 1.69                     | 0.75              |
| 1:M:97:HIS:ND1   | 1:M:123:ASP:OD2  | 2.20                     | 0.74              |
| 1:J:272:ASN:O    | 1:J:276:GLU:HG3  | 1.87                     | 0.74              |
| 1:F:130:SER:OG   | 1:F:132:SER:N    | 2.20                     | 0.74              |
| 1:M:126:THR:HG22 | 1:M:147:GLY:HA2  | 1.69                     | 0.74              |
| 1:L:109:ARG:HH11 | 1:L:109:ARG:CG   | 1.99                     | 0.74              |
| 1:I:169:ARG:NH1  | 1:I:234:VAL:O    | 2.20                     | 0.74              |
| 1:M:36:LEU:CD2   | 1:M:286:LEU:HD23 | 2.16                     | 0.74              |
| 1:L:198:ALA:O    | 1:L:202:GLU:HG2  | 1.86                     | 0.74              |
| 1:L:208:LEU:O    | 1:L:255:ARG:NH1  | 2.19                     | 0.74              |
| 1:A:159:ASP:OD1  | 1:A:161:LYS:HD3  | 1.87                     | 0.73              |
| 1:C:156:ARG:HH11 | 1:C:156:ARG:HG2  | 1.53                     | 0.73              |
| 1:G:84:LEU:O     | 1:G:109:ARG:NH2  | 2.21                     | 0.73              |
| 1:M:145:GLY:CA   | 1:M:156:ARG:HH11 | 2.00                     | 0.73              |
| 1:H:25:SER:O     | 1:H:29:TYR:HD2   | 1.71                     | 0.73              |
| 1:G:130:SER:HG   | 1:G:132:SER:N    | 1.85                     | 0.73              |
| 1:F:145:GLY:HA3  | 1:F:156:ARG:HD3  | 1.70                     | 0.73              |
| 1:L:33:LEU:O     | 1:L:37:GLU:HG3   | 1.88                     | 0.73              |
| 1:K:70:ILE:HD13  | 1:K:135:VAL:HG11 | 1.70                     | 0.73              |
| 1:D:244:HIS:O    | 1:D:248:GLU:HG3  | 1.89                     | 0.73              |
| 1:H:97:HIS:ND1   | 1:H:123:ASP:OD2  | 2.21                     | 0.73              |
| 1:I:278:LEU:HD12 | 1:I:281:LEU:HD12 | 1.71                     | 0.73              |
| 1:C:227:ALA:HB1  | 1:C:274:THR:HG23 | 1.69                     | 0.73              |
| 1:J:97:HIS:ND1   | 1:J:123:ASP:OD2  | 2.22                     | 0.73              |
| 1:G:146:LEU:HD23 | 1:G:146:LEU:N    | 2.04                     | 0.73              |
| 1:F:200:ILE:O    | 1:F:204:VAL:HG23 | 1.89                     | 0.73              |
| 1:F:125:ASN:O    | 1:F:138:MET:HB3  | 1.88                     | 0.72              |
| 1:E:149:PRO:O    | 1:E:153:GLU:HG2  | 1.89                     | 0.72              |
| 1:M:117:TRP:CD1  | 1:M:165:LEU:HD21 | 2.24                     | 0.72              |
| 1:C:83:ALA:CA    | 1:H:111:ARG:HH12 | 2.02                     | 0.72              |
| 1:H:129:THR:O    | 1:H:130:SER:HB2  | 1.89                     | 0.72              |
| 1:C:83:ALA:CA    | 1:H:111:ARG:NH1  | 2.52                     | 0.72              |
| 1:M:153:GLU:HG3  | 1:M:154:VAL:HG13 | 1.70                     | 0.72              |
| 1:D:273:ARG:HA   | 1:D:276:GLU:HG3  | 1.72                     | 0.72              |
| 1:M:84:LEU:HD13  | 1:M:88:VAL:HG11  | 1.71                     | 0.72              |
| 1:F:148:HIS:CD2  | 1:F:150:ARG:H    | 2.08                     | 0.72              |
| 1:D:104:VAL:HG22 | 1:D:214:HIS:CE1  | 2.25                     | 0.71              |
| 1:A:111:ARG:HH22 | 1:D:79:GLU:C     | 1.92                     | 0.71              |
| 1:M:80:ARG:CG    | 1:M:80:ARG:HH11  | 2.02                     | 0.71              |
| 1:H:11:MET:HE3   | 1:H:98:SER:HB2   | 1.73                     | 0.71              |
| 1:I:184:VAL:O    | 1:I:186:VAL:HG23 | 1.91                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:172:ASP:HB3  | 2:M:293:HOH:O    | 1.90                     | 0.71              |
| 1:J:99:LEU:C     | 1:J:99:LEU:HD12  | 2.11                     | 0.71              |
| 1:D:9:VAL:O      | 1:D:11:MET:N     | 2.23                     | 0.71              |
| 1:M:36:LEU:HD21  | 1:M:286:LEU:CD2  | 2.20                     | 0.71              |
| 1:H:66:TYR:O     | 1:H:70:ILE:HD13  | 1.91                     | 0.71              |
| 1:D:119:ASP:HB3  | 1:D:121:HIS:O    | 1.90                     | 0.71              |
| 1:J:201:ALA:HB1  | 1:J:249:ILE:HG21 | 1.73                     | 0.71              |
| 1:G:115:VAL:HB   | 1:G:163:VAL:HG22 | 1.71                     | 0.71              |
| 1:A:223:ASP:OD2  | 1:A:225:THR:HB   | 1.92                     | 0.70              |
| 1:K:164:VAL:CG2  | 1:K:208:LEU:HD11 | 2.21                     | 0.70              |
| 1:G:109:ARG:NH1  | 1:G:109:ARG:HG2  | 2.03                     | 0.70              |
| 1:D:214:HIS:CD2  | 1:D:258:SER:HB2  | 2.26                     | 0.70              |
| 1:H:101:MET:HA   | 1:H:143:LEU:HD21 | 1.73                     | 0.70              |
| 1:A:84:LEU:O     | 1:A:109:ARG:NH2  | 2.23                     | 0.70              |
| 1:K:214:HIS:HE1  | 1:K:260:ASP:OD2  | 1.73                     | 0.70              |
| 1:D:99:LEU:HD21  | 1:D:262:VAL:HG12 | 1.74                     | 0.70              |
| 1:C:119:ASP:OD2  | 1:C:123:ASP:OD2  | 2.10                     | 0.70              |
| 1:J:30:ALA:HB3   | 1:J:279:VAL:HG21 | 1.73                     | 0.70              |
| 1:K:118:VAL:HG23 | 1:K:216:SER:O    | 1.92                     | 0.70              |
| 1:I:119:ASP:OD2  | 1:I:123:ASP:OD2  | 2.10                     | 0.70              |
| 1:L:97:HIS:ND1   | 1:L:123:ASP:OD2  | 2.25                     | 0.70              |
| 1:G:111:ARG:HD3  | 1:G:112:ARG:H    | 1.56                     | 0.70              |
| 1:H:130:SER:HG   | 1:H:132:SER:N    | 1.89                     | 0.70              |
| 1:I:11:MET:CE    | 1:I:98:SER:HB2   | 2.22                     | 0.69              |
| 1:A:119:ASP:OD2  | 1:A:218:ASP:OD2  | 2.09                     | 0.69              |
| 1:D:129:THR:O    | 1:D:130:SER:HB2  | 1.91                     | 0.69              |
| 1:C:148:HIS:CD2  | 1:C:150:ARG:H    | 2.07                     | 0.69              |
| 1:F:169:ARG:HG3  | 1:F:234:VAL:HG11 | 1.74                     | 0.69              |
| 1:G:97:HIS:ND1   | 1:G:123:ASP:OD2  | 2.26                     | 0.69              |
| 1:A:220:ASP:OD2  | 2:A:293:HOH:O    | 2.10                     | 0.69              |
| 1:A:117:TRP:CE3  | 1:A:140:LEU:HD13 | 2.27                     | 0.69              |
| 1:M:190:HIS:HE1  | 1:M:194:ARG:HG3  | 1.57                     | 0.69              |
| 1:K:19:GLY:HA3   | 1:K:265:ASN:HD21 | 1.57                     | 0.69              |
| 1:I:12:ASP:OD2   | 1:I:19:GLY:HA2   | 1.92                     | 0.69              |
| 1:A:198:ALA:O    | 1:A:202:GLU:HG2  | 1.93                     | 0.69              |
| 1:A:79:GLU:CB    | 1:D:111:ARG:NH2  | 2.56                     | 0.69              |
| 1:M:80:ARG:HD2   | 1:M:80:ARG:O     | 1.93                     | 0.69              |
| 1:J:6:VAL:HG13   | 1:J:93:LEU:HD21  | 1.74                     | 0.69              |
| 1:J:119:ASP:OD2  | 1:J:123:ASP:OD2  | 2.11                     | 0.69              |
| 1:M:125:ASN:HB2  | 1:M:137:GLY:O    | 1.92                     | 0.68              |
| 1:L:149:PRO:O    | 1:L:153:GLU:HB3  | 1.93                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:109:ARG:HH11 | 1:A:109:ARG:HG2  | 1.56                     | 0.68              |
| 1:L:156:ARG:HG2  | 1:L:156:ARG:HH11 | 1.57                     | 0.68              |
| 1:E:239:THR:OG1  | 1:E:242:GLU:HB2  | 1.93                     | 0.68              |
| 1:J:66:TYR:HB3   | 1:J:70:ILE:CD1   | 2.23                     | 0.68              |
| 1:E:99:LEU:HD12  | 1:E:100:SER:N    | 2.08                     | 0.68              |
| 1:M:11:MET:HG2   | 1:M:96:ASP:HB2   | 1.75                     | 0.68              |
| 1:G:195:LEU:HD22 | 1:G:199:ARG:NH1  | 2.09                     | 0.68              |
| 1:J:66:TYR:HB3   | 1:J:70:ILE:HD11  | 1.74                     | 0.68              |
| 1:M:190:HIS:CE1  | 1:M:194:ARG:HG3  | 2.29                     | 0.68              |
| 1:K:78:LYS:HA    | 1:K:102:GLY:O    | 1.93                     | 0.68              |
| 1:J:211:LEU:O    | 1:J:255:ARG:NH1  | 2.25                     | 0.68              |
| 1:M:244:HIS:O    | 1:M:248:GLU:HG3  | 1.94                     | 0.68              |
| 1:J:125:ASN:HD21 | 1:J:175:GLU:HG3  | 1.58                     | 0.68              |
| 1:I:259:LEU:HD13 | 1:I:285:LEU:HD23 | 1.76                     | 0.68              |
| 1:L:119:ASP:OD1  | 1:L:121:HIS:ND1  | 2.27                     | 0.67              |
| 1:D:86:GLU:HG2   | 1:D:109:ARG:HH21 | 1.58                     | 0.67              |
| 1:I:179:LEU:HD22 | 1:I:186:VAL:HG21 | 1.77                     | 0.67              |
| 1:G:218:ASP:OD1  | 1:G:263:GLU:HG3  | 1.93                     | 0.67              |
| 1:J:164:VAL:HG11 | 1:J:204:VAL:CG2  | 2.25                     | 0.67              |
| 1:I:119:ASP:OD2  | 1:I:218:ASP:OD2  | 2.13                     | 0.67              |
| 1:M:124:PHE:HE2  | 1:M:178:LEU:HB3  | 1.60                     | 0.67              |
| 1:D:101:MET:HA   | 1:D:143:LEU:HD21 | 1.76                     | 0.67              |
| 1:F:223:ASP:OD2  | 1:F:225:THR:HB   | 1.93                     | 0.67              |
| 1:M:120:ALA:O    | 1:M:168:VAL:HA   | 1.95                     | 0.67              |
| 1:A:156:ARG:NH2  | 1:D:156:ARG:NH2  | 2.42                     | 0.67              |
| 1:H:84:LEU:O     | 1:H:85:PRO:O     | 2.12                     | 0.67              |
| 1:H:111:ARG:NE   | 1:H:112:ARG:H    | 1.92                     | 0.67              |
| 1:K:119:ASP:OD2  | 1:K:123:ASP:OD2  | 2.13                     | 0.67              |
| 1:J:148:HIS:HD2  | 1:J:150:ARG:HB2  | 1.59                     | 0.67              |
| 1:I:148:HIS:HD2  | 1:I:149:PRO:HD2  | 1.60                     | 0.67              |
| 1:E:240:TYR:HB3  | 2:E:306:HOH:O    | 1.95                     | 0.67              |
| 1:M:153:GLU:HG3  | 1:M:154:VAL:N    | 2.08                     | 0.67              |
| 1:J:177:ARG:HH11 | 1:J:177:ARG:HB3  | 1.59                     | 0.67              |
| 1:J:86:GLU:HG2   | 1:J:109:ARG:HE   | 1.60                     | 0.67              |
| 1:L:130:SER:OG   | 1:L:132:SER:N    | 2.27                     | 0.67              |
| 1:M:128:GLU:O    | 1:M:130:SER:N    | 2.27                     | 0.66              |
| 1:M:109:ARG:NH1  | 1:M:109:ARG:HG2  | 2.08                     | 0.66              |
| 1:A:119:ASP:OD2  | 1:A:123:ASP:OD2  | 2.13                     | 0.66              |
| 1:K:117:TRP:HB3  | 1:K:165:LEU:HD23 | 1.75                     | 0.66              |
| 1:K:41:TYR:OH    | 1:K:286:LEU:O    | 2.12                     | 0.66              |
| 1:D:43:VAL:HG12  | 1:D:44:GLU:N     | 2.10                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:125:ASN:ND2  | 1:M:129:THR:OG1  | 2.28                     | 0.66              |
| 1:L:140:LEU:HD21 | 1:L:163:VAL:HG11 | 1.77                     | 0.66              |
| 1:M:12:ASP:OD2   | 1:M:19:GLY:HA2   | 1.95                     | 0.66              |
| 1:K:9:VAL:HB     | 1:K:99:LEU:HD22  | 1.77                     | 0.66              |
| 1:C:117:TRP:HB3  | 1:C:165:LEU:HD23 | 1.78                     | 0.66              |
| 1:L:96:ASP:HB3   | 1:L:98:SER:OG    | 1.94                     | 0.66              |
| 1:I:25:SER:HB3   | 1:M:22:MET:CE    | 2.26                     | 0.66              |
| 1:H:111:ARG:NE   | 1:H:111:ARG:CA   | 2.58                     | 0.66              |
| 1:M:117:TRP:HD1  | 1:M:165:LEU:HD21 | 1.61                     | 0.66              |
| 1:K:211:LEU:O    | 1:K:255:ARG:HD2  | 1.96                     | 0.66              |
| 1:K:214:HIS:CE1  | 1:K:260:ASP:OD2  | 2.49                     | 0.66              |
| 1:G:11:MET:CE    | 1:G:98:SER:HB2   | 2.24                     | 0.66              |
| 1:L:189:MET:HA   | 1:L:192:VAL:HG23 | 1.77                     | 0.66              |
| 1:D:138:MET:H    | 1:D:139:PRO:HD3  | 1.60                     | 0.66              |
| 1:F:259:LEU:HD13 | 1:F:285:LEU:CD2  | 2.25                     | 0.66              |
| 1:L:129:THR:O    | 1:L:130:SER:HB3  | 1.96                     | 0.66              |
| 1:M:165:LEU:HB2  | 1:M:186:VAL:HG22 | 1.77                     | 0.66              |
| 1:I:97:HIS:CD2   | 1:I:262:VAL:HG21 | 2.31                     | 0.66              |
| 1:D:119:ASP:OD2  | 1:D:123:ASP:OD2  | 2.13                     | 0.66              |
| 1:L:239:THR:OG1  | 1:L:242:GLU:HG3  | 1.96                     | 0.66              |
| 1:M:29:TYR:C     | 1:M:31:ARG:H     | 1.98                     | 0.66              |
| 1:E:4:VAL:HG11   | 1:E:36:LEU:HD13  | 1.77                     | 0.66              |
| 1:I:81:LEU:HA    | 1:I:84:LEU:HD12  | 1.77                     | 0.66              |
| 1:H:22:MET:SD    | 1:H:267:ILE:HD13 | 2.35                     | 0.66              |
| 1:H:33:LEU:HG    | 1:H:43:VAL:HG11  | 1.78                     | 0.66              |
| 1:E:138:MET:H    | 1:E:139:PRO:CD   | 2.10                     | 0.65              |
| 1:I:169:ARG:NH2  | 1:I:221:VAL:O    | 2.28                     | 0.65              |
| 1:K:72:ALA:O     | 1:K:76:VAL:HG23  | 1.96                     | 0.65              |
| 1:A:11:MET:CE    | 1:A:98:SER:HB2   | 2.26                     | 0.65              |
| 1:L:169:ARG:HD2  | 1:L:234:VAL:HB   | 1.77                     | 0.65              |
| 1:A:130:SER:OG   | 1:A:132:SER:N    | 2.29                     | 0.65              |
| 1:G:11:MET:HE1   | 1:G:98:SER:HB2   | 1.77                     | 0.65              |
| 1:C:86:GLU:HG2   | 1:C:109:ARG:NE   | 2.11                     | 0.65              |
| 1:J:129:THR:O    | 1:J:130:SER:HB2  | 1.96                     | 0.65              |
| 1:H:129:THR:O    | 1:H:130:SER:CB   | 2.44                     | 0.65              |
| 1:A:169:ARG:HG3  | 1:A:234:VAL:HG11 | 1.79                     | 0.65              |
| 1:L:97:HIS:CD2   | 1:L:262:VAL:HG21 | 2.32                     | 0.65              |
| 1:L:3:ARG:NH2    | 1:L:88:VAL:N     | 2.44                     | 0.65              |
| 1:L:201:ALA:HB1  | 1:L:249:ILE:HG21 | 1.78                     | 0.65              |
| 1:F:149:PRO:HA   | 1:F:152:THR:OG1  | 1.97                     | 0.65              |
| 1:I:109:ARG:HG2  | 1:I:109:ARG:NH1  | 2.12                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:244:HIS:O    | 1:G:248:GLU:HG3  | 1.97                     | 0.65              |
| 1:K:239:THR:OG1  | 1:K:242:GLU:HG3  | 1.96                     | 0.65              |
| 1:M:31:ARG:O     | 1:M:35:GLN:HG3   | 1.96                     | 0.65              |
| 1:E:290:ILE:HD12 | 1:E:290:ILE:H    | 1.62                     | 0.65              |
| 1:D:11:MET:HE1   | 1:D:98:SER:HB2   | 1.76                     | 0.65              |
| 1:M:35:GLN:HB3   | 1:M:283:LEU:HD11 | 1.79                     | 0.65              |
| 1:K:71:ARG:NH2   | 1:K:153:GLU:OE2  | 2.30                     | 0.64              |
| 1:J:138:MET:N    | 1:J:139:PRO:CD   | 2.60                     | 0.64              |
| 1:H:222:LEU:HD13 | 1:H:277:MET:HE2  | 1.78                     | 0.64              |
| 1:A:256:VAL:HG21 | 1:A:285:LEU:HD11 | 1.79                     | 0.64              |
| 1:A:111:ARG:HH22 | 1:D:79:GLU:CA    | 2.10                     | 0.64              |
| 1:M:145:GLY:HA3  | 1:M:156:ARG:NH1  | 2.08                     | 0.64              |
| 1:K:218:ASP:HA   | 1:K:262:VAL:HG23 | 1.78                     | 0.64              |
| 1:E:149:PRO:HA   | 1:E:152:THR:OG1  | 1.97                     | 0.64              |
| 1:L:218:ASP:OD1  | 1:L:220:ASP:OD2  | 2.15                     | 0.64              |
| 1:E:31:ARG:NH2   | 1:E:34:GLU:HG2   | 2.12                     | 0.64              |
| 1:C:83:ALA:HA    | 1:H:111:ARG:NH1  | 2.12                     | 0.64              |
| 1:K:94:GLY:HA2   | 1:K:99:LEU:HD21  | 1.80                     | 0.64              |
| 1:I:164:VAL:HG11 | 1:I:204:VAL:HG22 | 1.79                     | 0.64              |
| 1:C:248:GLU:OE1  | 1:I:190:HIS:HD2  | 1.81                     | 0.64              |
| 1:H:130:SER:OG   | 1:H:132:SER:N    | 2.31                     | 0.64              |
| 1:I:85:PRO:O     | 1:I:88:VAL:HG23  | 1.97                     | 0.64              |
| 1:G:169:ARG:NH2  | 1:G:221:VAL:O    | 2.31                     | 0.64              |
| 1:J:101:MET:HA   | 1:J:143:LEU:HD21 | 1.79                     | 0.64              |
| 1:F:98:SER:HA    | 1:F:139:PRO:HG3  | 1.79                     | 0.64              |
| 1:D:214:HIS:HD2  | 1:D:258:SER:HB2  | 1.62                     | 0.64              |
| 1:K:205:LEU:O    | 1:K:209:GLN:N    | 2.30                     | 0.64              |
| 1:J:7:VAL:CG1    | 1:J:92:VAL:HG22  | 2.28                     | 0.64              |
| 1:D:111:ARG:HE   | 1:D:112:ARG:N    | 1.96                     | 0.64              |
| 1:E:197:VAL:HG21 | 1:E:242:GLU:CG   | 2.27                     | 0.64              |
| 1:E:101:MET:HA   | 1:E:143:LEU:HD21 | 1.80                     | 0.64              |
| 1:I:67:LEU:C     | 1:I:67:LEU:CD2   | 2.66                     | 0.64              |
| 1:J:156:ARG:HH11 | 1:J:156:ARG:CG   | 2.10                     | 0.64              |
| 1:A:156:ARG:NH2  | 1:D:156:ARG:HH21 | 1.95                     | 0.64              |
| 1:D:71:ARG:O     | 1:D:75:LEU:HB2   | 1.98                     | 0.64              |
| 1:H:171:LEU:HB2  | 1:H:176:LYS:HE2  | 1.80                     | 0.64              |
| 1:E:80:ARG:HD3   | 2:E:293:HOH:O    | 1.97                     | 0.64              |
| 1:E:138:MET:N    | 1:E:139:PRO:CD   | 2.61                     | 0.63              |
| 1:E:6:VAL:HG22   | 1:E:91:ILE:HB    | 1.80                     | 0.63              |
| 1:I:31:ARG:HD2   | 2:I:294:HOH:O    | 1.97                     | 0.63              |
| 1:J:169:ARG:NH1  | 1:J:234:VAL:O    | 2.29                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:226:LEU:HD21 | 1:K:240:TYR:N    | 2.13                     | 0.63              |
| 1:L:112:ARG:NH1  | 1:L:211:LEU:HD21 | 2.12                     | 0.63              |
| 1:L:108:ALA:C    | 1:L:109:ARG:HG3  | 2.19                     | 0.63              |
| 1:L:130:SER:HG   | 1:L:132:SER:N    | 1.94                     | 0.63              |
| 1:L:164:VAL:HG13 | 1:L:185:ARG:HB3  | 1.79                     | 0.63              |
| 1:E:156:ARG:HH11 | 1:E:156:ARG:HG2  | 1.63                     | 0.63              |
| 1:M:126:THR:OG1  | 1:M:129:THR:HG23 | 1.98                     | 0.63              |
| 1:C:271:ARG:HH21 | 1:K:228:PRO:HB2  | 1.61                     | 0.63              |
| 1:G:138:MET:N    | 1:G:139:PRO:CD   | 2.61                     | 0.63              |
| 1:K:243:ALA:HB1  | 1:K:281:LEU:HD11 | 1.79                     | 0.63              |
| 1:A:109:ARG:NH1  | 1:A:109:ARG:HG2  | 2.11                     | 0.63              |
| 1:A:226:LEU:HD21 | 1:A:240:TYR:HB2  | 1.80                     | 0.63              |
| 1:K:159:ASP:O    | 1:K:161:LYS:N    | 2.32                     | 0.63              |
| 1:A:71:ARG:O     | 1:A:75:LEU:HB2   | 1.97                     | 0.63              |
| 1:M:20:VAL:HG12  | 1:M:264:VAL:O    | 1.99                     | 0.63              |
| 1:C:119:ASP:HB3  | 1:C:121:HIS:O    | 1.98                     | 0.63              |
| 1:D:259:LEU:HD13 | 1:D:285:LEU:HD23 | 1.79                     | 0.63              |
| 1:F:115:VAL:HG23 | 1:F:158:VAL:HG21 | 1.81                     | 0.63              |
| 1:L:93:LEU:CD2   | 1:L:261:LEU:HD12 | 2.29                     | 0.63              |
| 1:L:27:LEU:HD21  | 1:L:264:VAL:HG21 | 1.81                     | 0.63              |
| 1:K:192:VAL:HA   | 1:K:200:ILE:HD11 | 1.80                     | 0.63              |
| 1:G:119:ASP:OD2  | 1:G:218:ASP:OD2  | 2.17                     | 0.62              |
| 1:M:259:LEU:HD13 | 1:M:285:LEU:CD2  | 2.28                     | 0.62              |
| 1:H:244:HIS:O    | 1:H:248:GLU:HG3  | 1.99                     | 0.62              |
| 1:M:138:MET:N    | 1:M:139:PRO:CD   | 2.60                     | 0.62              |
| 1:I:216:SER:HA   | 1:I:260:ASP:HB2  | 1.80                     | 0.62              |
| 1:E:51:VAL:O     | 1:E:51:VAL:HG12  | 1.99                     | 0.62              |
| 1:L:247:MET:HG3  | 1:L:281:LEU:O    | 1.99                     | 0.62              |
| 1:F:99:LEU:HD12  | 1:F:100:SER:N    | 2.14                     | 0.62              |
| 1:A:104:VAL:HG22 | 1:A:214:HIS:CE1  | 2.33                     | 0.62              |
| 1:E:119:ASP:HB3  | 1:E:121:HIS:O    | 1.99                     | 0.62              |
| 1:I:49:VAL:HG21  | 1:I:77:LEU:HD13  | 1.81                     | 0.62              |
| 1:D:117:TRP:CE3  | 1:D:140:LEU:HD13 | 2.35                     | 0.62              |
| 1:J:104:VAL:HB   | 1:J:143:LEU:HD22 | 1.81                     | 0.62              |
| 1:A:67:LEU:HD11  | 1:A:148:HIS:CD2  | 2.35                     | 0.62              |
| 1:J:148:HIS:CD2  | 1:J:150:ARG:HB2  | 2.34                     | 0.62              |
| 1:A:119:ASP:HA   | 1:A:218:ASP:HB3  | 1.82                     | 0.62              |
| 1:E:256:VAL:HG11 | 1:E:285:LEU:HD11 | 1.80                     | 0.62              |
| 1:A:69:GLU:OE1   | 1:A:69:GLU:N     | 2.31                     | 0.62              |
| 1:K:176:LYS:HB3  | 1:M:291:PHE:HE2  | 1.64                     | 0.62              |
| 1:K:165:LEU:HD12 | 1:K:186:VAL:CG2  | 2.29                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:25:SER:O     | 1:A:29:TYR:HD2   | 1.81                     | 0.62              |
| 1:A:164:VAL:HG11 | 1:A:204:VAL:HG22 | 1.81                     | 0.62              |
| 1:I:126:THR:HG23 | 1:I:178:LEU:HD13 | 1.81                     | 0.62              |
| 1:J:46:LEU:HD22  | 1:J:80:ARG:NH2   | 2.15                     | 0.62              |
| 1:F:13:LEU:HB2   | 1:F:70:ILE:HD11  | 1.82                     | 0.62              |
| 1:D:138:MET:N    | 1:D:139:PRO:CD   | 2.62                     | 0.62              |
| 1:L:12:ASP:HA    | 1:L:96:ASP:OD1   | 1.99                     | 0.62              |
| 1:M:164:VAL:HG11 | 1:M:204:VAL:CG2  | 2.30                     | 0.61              |
| 1:I:198:ALA:O    | 1:I:202:GLU:HG2  | 1.99                     | 0.61              |
| 1:K:100:SER:HA   | 1:K:103:SER:OG   | 2.00                     | 0.61              |
| 1:D:223:ASP:OD2  | 1:D:225:THR:HG22 | 2.00                     | 0.61              |
| 1:L:119:ASP:HA   | 1:L:218:ASP:HB3  | 1.81                     | 0.61              |
| 1:L:169:ARG:HG3  | 1:L:234:VAL:HG11 | 1.83                     | 0.61              |
| 1:H:94:GLY:HA3   | 1:H:99:LEU:CD2   | 2.30                     | 0.61              |
| 1:F:179:LEU:HD13 | 1:F:186:VAL:HG21 | 1.82                     | 0.61              |
| 1:M:30:ALA:HB3   | 1:M:279:VAL:HG21 | 1.83                     | 0.61              |
| 1:A:138:MET:N    | 1:A:139:PRO:CD   | 2.63                     | 0.61              |
| 1:A:169:ARG:HA   | 1:E:290:ILE:HG21 | 1.82                     | 0.61              |
| 1:C:130:SER:HG   | 1:C:132:SER:N    | 1.98                     | 0.61              |
| 1:K:101:MET:HA   | 1:K:143:LEU:HD21 | 1.83                     | 0.61              |
| 1:G:12:ASP:C     | 1:G:13:LEU:HD23  | 2.19                     | 0.61              |
| 1:M:4:VAL:HG23   | 1:M:41:TYR:HD1   | 1.65                     | 0.61              |
| 1:E:129:THR:O    | 1:E:130:SER:CB   | 2.49                     | 0.61              |
| 1:D:94:GLY:HA3   | 1:D:99:LEU:CD2   | 2.30                     | 0.61              |
| 1:G:195:LEU:HD22 | 1:G:199:ARG:HH11 | 1.66                     | 0.61              |
| 1:H:201:ALA:HB1  | 1:H:249:ILE:HG21 | 1.83                     | 0.61              |
| 1:I:248:GLU:O    | 1:I:252:GLU:HG3  | 2.00                     | 0.61              |
| 1:I:123:ASP:HB3  | 1:I:139:PRO:HG2  | 1.81                     | 0.61              |
| 1:M:244:HIS:CE1  | 1:M:281:LEU:HD23 | 2.35                     | 0.61              |
| 1:A:79:GLU:HG2   | 1:D:111:ARG:NH2  | 2.15                     | 0.61              |
| 1:C:80:ARG:O     | 1:C:83:ALA:HB3   | 2.00                     | 0.61              |
| 1:F:71:ARG:HD3   | 2:F:299:HOH:O    | 2.00                     | 0.61              |
| 1:J:119:ASP:HA   | 1:J:218:ASP:HB3  | 1.83                     | 0.61              |
| 1:A:94:GLY:HA3   | 1:A:99:LEU:CD2   | 2.31                     | 0.61              |
| 1:M:12:ASP:C     | 1:M:13:LEU:HD23  | 2.22                     | 0.60              |
| 1:K:113:VAL:CG1  | 1:K:212:PRO:HG2  | 2.25                     | 0.60              |
| 1:M:84:LEU:CD1   | 1:M:88:VAL:HG11  | 2.29                     | 0.60              |
| 1:F:138:MET:H    | 1:F:139:PRO:HD3  | 1.64                     | 0.60              |
| 1:M:31:ARG:HB2   | 1:M:31:ARG:HH11  | 1.66                     | 0.60              |
| 1:D:81:LEU:O     | 1:D:84:LEU:HD12  | 2.01                     | 0.60              |
| 1:G:2:GLU:HB2    | 2:G:294:HOH:O    | 2.00                     | 0.60              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:84:LEU:O    | 1:H:109:ARG:NH2  | 2.33                     | 0.60              |
| 1:E:130:SER:OG  | 1:E:132:SER:N    | 2.34                     | 0.60              |
| 1:L:11:MET:HG3  | 1:L:12:ASP:N     | 2.16                     | 0.60              |
| 1:K:124:PHE:HD1 | 1:K:140:LEU:HB3  | 1.66                     | 0.60              |
| 1:E:148:HIS:CD2 | 1:E:150:ARG:HB2  | 2.36                     | 0.60              |
| 1:H:111:ARG:CD  | 1:H:112:ARG:N    | 2.51                     | 0.60              |
| 1:L:112:ARG:HD3 | 1:L:211:LEU:CD2  | 2.31                     | 0.60              |
| 1:D:129:THR:O   | 1:D:130:SER:CB   | 2.49                     | 0.60              |
| 1:A:97:HIS:CE1  | 1:A:117:TRP:CZ2  | 2.89                     | 0.60              |
| 1:K:169:ARG:NH1 | 1:K:234:VAL:O    | 2.34                     | 0.60              |
| 1:C:25:SER:O    | 1:C:29:TYR:HD2   | 1.84                     | 0.60              |
| 1:D:22:MET:HE3  | 1:J:25:SER:HB2   | 1.82                     | 0.60              |
| 1:G:138:MET:H   | 1:G:139:PRO:CD   | 2.14                     | 0.60              |
| 1:G:119:ASP:HB3 | 1:G:121:HIS:O    | 2.02                     | 0.60              |
| 1:H:138:MET:N   | 1:H:139:PRO:HD2  | 2.16                     | 0.60              |
| 1:L:119:ASP:OD2 | 1:L:123:ASP:OD2  | 2.19                     | 0.60              |
| 1:I:149:PRO:HA  | 1:I:152:THR:OG1  | 2.02                     | 0.60              |
| 1:J:35:GLN:HA   | 1:J:38:ASP:OD2   | 2.01                     | 0.60              |
| 1:L:209:GLN:HA  | 1:L:255:ARG:HH22 | 1.65                     | 0.60              |
| 1:L:3:ARG:NH2   | 1:L:87:GLY:C     | 2.54                     | 0.60              |
| 1:K:124:PHE:HD2 | 1:K:179:LEU:HG   | 1.67                     | 0.60              |
| 1:C:225:THR:CG2 | 1:C:226:LEU:N    | 2.63                     | 0.60              |
| 1:J:269:ASP:OD1 | 1:J:270:GLU:N    | 2.30                     | 0.60              |
| 1:M:117:TRP:CE3 | 1:M:140:LEU:HD13 | 2.37                     | 0.60              |
| 1:J:122:ALA:O   | 1:J:123:ASP:C    | 2.39                     | 0.60              |
| 1:A:68:GLU:CD   | 1:A:150:ARG:HH21 | 2.05                     | 0.60              |
| 1:I:37:GLU:HG2  | 1:I:43:VAL:HG23  | 1.83                     | 0.60              |
| 1:G:262:VAL:O   | 1:G:263:GLU:HB2  | 2.01                     | 0.60              |
| 1:L:4:VAL:HG13  | 1:L:91:ILE:HD11  | 1.84                     | 0.60              |
| 1:F:99:LEU:C    | 1:F:99:LEU:HD12  | 2.22                     | 0.60              |
| 1:H:169:ARG:NH2 | 1:H:221:VAL:O    | 2.35                     | 0.60              |
| 1:H:111:ARG:HE  | 1:H:111:ARG:CA   | 2.10                     | 0.60              |
| 1:K:111:ARG:HD3 | 1:K:112:ARG:N    | 2.12                     | 0.60              |
| 1:L:165:LEU:HB2 | 1:L:186:VAL:HG22 | 1.83                     | 0.60              |
| 1:C:218:ASP:O   | 1:C:221:VAL:HG12 | 2.02                     | 0.60              |
| 1:C:125:ASN:ND2 | 1:C:175:GLU:HG3  | 2.16                     | 0.60              |
| 1:C:32:LEU:O    | 1:C:36:LEU:HD12  | 2.02                     | 0.60              |
| 1:C:119:ASP:OD2 | 1:C:218:ASP:OD2  | 2.20                     | 0.59              |
| 1:A:153:GLU:HA  | 1:D:156:ARG:CZ   | 2.31                     | 0.59              |
| 1:H:71:ARG:NH2  | 1:H:154:VAL:HG11 | 2.17                     | 0.59              |
| 1:J:81:LEU:HD23 | 1:J:84:LEU:HD11  | 1.82                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:25:SER:O     | 1:K:29:TYR:HD2   | 1.85                     | 0.59              |
| 1:F:112:ARG:CZ   | 1:F:211:LEU:HD21 | 2.32                     | 0.59              |
| 1:J:261:LEU:HD11 | 1:J:282:ALA:HB2  | 1.84                     | 0.59              |
| 1:L:33:LEU:CD2   | 1:L:43:VAL:HB    | 2.30                     | 0.59              |
| 1:E:33:LEU:HD23  | 1:E:43:VAL:HB    | 1.84                     | 0.59              |
| 1:D:92:VAL:HG11  | 1:D:99:LEU:HD13  | 1.84                     | 0.59              |
| 1:J:30:ALA:CB    | 1:J:279:VAL:HG21 | 2.33                     | 0.59              |
| 1:M:194:ARG:HG2  | 1:M:194:ARG:HH11 | 1.67                     | 0.59              |
| 1:C:99:LEU:C     | 1:C:99:LEU:HD12  | 2.23                     | 0.59              |
| 1:C:12:ASP:OD2   | 1:C:19:GLY:HA2   | 2.02                     | 0.59              |
| 1:J:22:MET:SD    | 1:J:267:ILE:HD12 | 2.43                     | 0.59              |
| 1:C:223:ASP:OD2  | 1:C:225:THR:HB   | 2.02                     | 0.59              |
| 1:C:225:THR:HG22 | 1:C:226:LEU:N    | 2.18                     | 0.59              |
| 1:A:239:THR:OG1  | 1:A:242:GLU:HG3  | 2.03                     | 0.59              |
| 1:D:97:HIS:CE1   | 1:D:119:ASP:OD2  | 2.56                     | 0.59              |
| 1:J:177:ARG:NH1  | 1:J:177:ARG:HB3  | 2.17                     | 0.59              |
| 1:I:99:LEU:HD12  | 1:I:99:LEU:C     | 2.22                     | 0.59              |
| 1:K:67:LEU:HD23  | 1:K:67:LEU:C     | 2.23                     | 0.59              |
| 1:H:149:PRO:O    | 1:H:153:GLU:HG2  | 2.03                     | 0.59              |
| 1:M:11:MET:SD    | 1:M:70:ILE:HD13  | 2.42                     | 0.59              |
| 1:L:37:GLU:HG2   | 1:L:43:VAL:CG2   | 2.32                     | 0.59              |
| 1:A:138:MET:H    | 1:A:139:PRO:HD2  | 1.66                     | 0.59              |
| 1:L:156:ARG:HG2  | 1:L:156:ARG:NH1  | 2.16                     | 0.59              |
| 1:E:119:ASP:OD2  | 1:E:218:ASP:OD2  | 2.21                     | 0.59              |
| 1:K:49:VAL:O     | 1:K:51:VAL:HG23  | 2.02                     | 0.59              |
| 1:L:91:ILE:HD13  | 1:L:91:ILE:N     | 2.18                     | 0.59              |
| 1:D:153:GLU:HG3  | 1:D:154:VAL:HG13 | 1.84                     | 0.59              |
| 1:K:104:VAL:HG22 | 1:K:214:HIS:CE1  | 2.38                     | 0.58              |
| 1:E:97:HIS:CD2   | 1:E:262:VAL:HG21 | 2.38                     | 0.58              |
| 1:G:129:THR:O    | 1:G:130:SER:HB3  | 2.03                     | 0.58              |
| 1:D:97:HIS:CD2   | 1:D:262:VAL:HG21 | 2.38                     | 0.58              |
| 1:E:148:HIS:HD2  | 1:E:150:ARG:H    | 1.51                     | 0.58              |
| 1:C:96:ASP:HA    | 1:C:263:GLU:OE2  | 2.03                     | 0.58              |
| 1:L:138:MET:N    | 1:L:139:PRO:CD   | 2.60                     | 0.58              |
| 1:I:125:ASN:O    | 1:I:138:MET:HG2  | 2.03                     | 0.58              |
| 1:M:31:ARG:CB    | 1:M:31:ARG:HH11  | 2.15                     | 0.58              |
| 1:G:223:ASP:OD2  | 1:G:225:THR:HB   | 2.02                     | 0.58              |
| 1:K:119:ASP:HB3  | 1:K:121:HIS:O    | 2.04                     | 0.58              |
| 1:E:145:GLY:C    | 1:E:146:LEU:HD23 | 2.23                     | 0.58              |
| 1:D:138:MET:N    | 1:D:139:PRO:HD3  | 2.17                     | 0.58              |
| 1:I:259:LEU:HG   | 1:I:260:ASP:N    | 2.18                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:129:THR:O    | 1:L:130:SER:CB   | 2.51                     | 0.58              |
| 1:L:129:THR:CG2  | 1:L:174:GLY:HA3  | 2.34                     | 0.58              |
| 1:I:94:GLY:HA3   | 1:I:99:LEU:HD21  | 1.86                     | 0.58              |
| 1:A:161:LYS:H    | 1:A:161:LYS:HD3  | 1.67                     | 0.58              |
| 1:F:214:HIS:HE1  | 1:F:260:ASP:OD2  | 1.86                     | 0.58              |
| 1:L:104:VAL:HB   | 1:L:143:LEU:HD21 | 1.84                     | 0.58              |
| 1:M:156:ARG:O    | 1:M:157:ALA:HB2  | 2.04                     | 0.58              |
| 1:L:165:LEU:HD12 | 1:L:186:VAL:HG22 | 1.85                     | 0.58              |
| 1:E:119:ASP:OD2  | 1:E:123:ASP:OD2  | 2.20                     | 0.58              |
| 1:M:31:ARG:CB    | 1:M:31:ARG:NH1   | 2.66                     | 0.58              |
| 1:M:253:SER:O    | 1:M:255:ARG:HG3  | 2.02                     | 0.58              |
| 1:J:34:GLU:N     | 1:J:34:GLU:OE1   | 2.36                     | 0.58              |
| 1:F:13:LEU:HD22  | 1:F:66:TYR:CG    | 2.38                     | 0.58              |
| 1:H:94:GLY:HA3   | 1:H:99:LEU:HD21  | 1.84                     | 0.58              |
| 1:M:164:VAL:HG11 | 1:M:204:VAL:HG22 | 1.84                     | 0.58              |
| 1:K:169:ARG:HG3  | 1:K:234:VAL:HG11 | 1.85                     | 0.58              |
| 1:M:145:GLY:HA2  | 1:M:156:ARG:HG2  | 1.86                     | 0.58              |
| 1:A:82:ALA:HA    | 1:A:109:ARG:NH1  | 2.19                     | 0.58              |
| 1:E:99:LEU:HD12  | 1:E:99:LEU:C     | 2.23                     | 0.58              |
| 1:K:159:ASP:HB3  | 1:K:162:ASP:OD1  | 2.03                     | 0.58              |
| 1:H:270:GLU:O    | 1:H:273:ARG:HG2  | 2.03                     | 0.58              |
| 1:M:2:GLU:OE2    | 1:M:3:ARG:HG3    | 2.04                     | 0.58              |
| 1:I:232:THR:O    | 1:I:234:VAL:HG23 | 2.04                     | 0.58              |
| 1:M:124:PHE:HA   | 1:M:141:ALA:HB2  | 1.86                     | 0.58              |
| 1:L:220:ASP:O    | 1:L:220:ASP:OD1  | 2.22                     | 0.58              |
| 1:A:215:VAL:O    | 1:A:259:LEU:HD12 | 2.04                     | 0.58              |
| 1:H:144:SER:HB3  | 1:H:160:PRO:HG3  | 1.86                     | 0.58              |
| 1:D:164:VAL:HG11 | 1:D:204:VAL:HG22 | 1.85                     | 0.58              |
| 1:C:30:ALA:HB3   | 1:C:279:VAL:HG21 | 1.85                     | 0.58              |
| 1:C:161:LYS:HD3  | 2:C:296:HOH:O    | 2.04                     | 0.58              |
| 1:C:214:HIS:HE1  | 1:C:260:ASP:OD2  | 1.87                     | 0.58              |
| 1:E:69:GLU:N     | 1:E:69:GLU:OE1   | 2.37                     | 0.58              |
| 1:M:22:MET:HB2   | 1:M:266:PRO:HG3  | 1.84                     | 0.57              |
| 1:K:169:ARG:NH2  | 1:K:237:GLY:HA3  | 2.19                     | 0.57              |
| 1:H:145:GLY:C    | 1:H:146:LEU:HD23 | 2.25                     | 0.57              |
| 1:L:118:VAL:HB   | 1:L:217:LEU:CD1  | 2.34                     | 0.57              |
| 1:H:12:ASP:O     | 1:H:12:ASP:OD1   | 2.21                     | 0.57              |
| 1:D:169:ARG:NH1  | 1:D:234:VAL:O    | 2.37                     | 0.57              |
| 1:I:36:LEU:CD2   | 1:I:286:LEU:HD23 | 2.32                     | 0.57              |
| 1:L:153:GLU:HG2  | 1:L:154:VAL:CG1  | 2.34                     | 0.57              |
| 1:G:10:PRO:HG3   | 1:G:48:ASP:OD2   | 2.04                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:24:PRO:HD3   | 1:F:94:GLY:O     | 2.04                     | 0.57              |
| 1:K:192:VAL:HA   | 1:K:200:ILE:CD1  | 2.35                     | 0.57              |
| 1:G:68:GLU:OE1   | 1:G:150:ARG:NH2  | 2.26                     | 0.57              |
| 1:L:148:HIS:HD2  | 1:L:150:ARG:HB2  | 1.69                     | 0.57              |
| 1:G:239:THR:OG1  | 1:G:242:GLU:HG3  | 2.04                     | 0.57              |
| 1:C:156:ARG:HG2  | 1:C:156:ARG:NH1  | 2.18                     | 0.57              |
| 1:L:153:GLU:HG2  | 1:L:154:VAL:HG13 | 1.85                     | 0.57              |
| 1:E:273:ARG:O    | 1:E:277:MET:HG3  | 2.04                     | 0.57              |
| 1:I:31:ARG:O     | 1:I:35:GLN:HG3   | 2.04                     | 0.57              |
| 1:K:159:ASP:C    | 1:K:161:LYS:H    | 2.06                     | 0.57              |
| 1:C:198:ALA:O    | 1:C:202:GLU:HG2  | 2.05                     | 0.57              |
| 1:F:111:ARG:HH22 | 1:G:249:ILE:HG23 | 1.70                     | 0.57              |
| 1:M:108:ALA:HB2  | 1:M:113:VAL:HG21 | 1.86                     | 0.57              |
| 1:L:89:PHE:HZ    | 1:L:256:VAL:HG12 | 1.69                     | 0.57              |
| 1:D:118:VAL:HG12 | 1:D:221:VAL:HG11 | 1.87                     | 0.57              |
| 1:H:156:ARG:HH11 | 1:H:156:ARG:HG2  | 1.69                     | 0.57              |
| 1:M:71:ARG:HG3   | 1:M:155:PHE:HE2  | 1.68                     | 0.57              |
| 1:E:190:HIS:O    | 1:E:194:ARG:HB2  | 2.05                     | 0.57              |
| 1:E:244:HIS:O    | 1:E:248:GLU:HG3  | 2.05                     | 0.57              |
| 1:M:129:THR:O    | 1:M:130:SER:CB   | 2.53                     | 0.57              |
| 1:E:2:GLU:O      | 1:E:42:THR:HG23  | 2.05                     | 0.57              |
| 1:G:24:PRO:O     | 1:G:28:ARG:HG3   | 2.04                     | 0.57              |
| 1:M:270:GLU:O    | 1:M:273:ARG:HG2  | 2.04                     | 0.57              |
| 1:K:74:ALA:O     | 1:K:77:LEU:HB3   | 2.05                     | 0.56              |
| 1:I:187:TYR:CD1  | 1:I:200:ILE:HD12 | 2.39                     | 0.56              |
| 1:G:25:SER:O     | 1:G:29:TYR:HD2   | 1.88                     | 0.56              |
| 1:G:138:MET:H    | 1:G:139:PRO:HD2  | 1.68                     | 0.56              |
| 1:I:104:VAL:HG22 | 1:I:214:HIS:ND1  | 2.20                     | 0.56              |
| 1:I:190:HIS:CE1  | 1:I:194:ARG:HE   | 2.24                     | 0.56              |
| 1:E:177:ARG:HH11 | 1:E:177:ARG:HB3  | 1.69                     | 0.56              |
| 1:I:67:LEU:HD23  | 1:I:67:LEU:O     | 2.04                     | 0.56              |
| 1:M:97:HIS:CE1   | 1:M:119:ASP:OD2  | 2.57                     | 0.56              |
| 1:G:109:ARG:HH11 | 1:G:109:ARG:CG   | 2.16                     | 0.56              |
| 1:J:52:SER:O     | 1:J:69:GLU:HB3   | 2.06                     | 0.56              |
| 1:G:81:LEU:HD13  | 1:G:107:ALA:HB2  | 1.86                     | 0.56              |
| 1:M:211:LEU:CB   | 2:M:296:HOH:O    | 2.47                     | 0.56              |
| 1:H:119:ASP:OD2  | 1:H:218:ASP:OD2  | 2.24                     | 0.56              |
| 1:A:94:GLY:HA3   | 1:A:99:LEU:HD21  | 1.88                     | 0.56              |
| 1:E:177:ARG:HB3  | 1:E:177:ARG:NH1  | 2.21                     | 0.56              |
| 1:M:239:THR:OG1  | 1:M:242:GLU:HG3  | 2.05                     | 0.56              |
| 1:C:83:ALA:C     | 1:H:111:ARG:NH1  | 2.53                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:283:LEU:HD23 | 1:M:283:LEU:N    | 2.21                     | 0.56              |
| 1:A:148:HIS:HD2  | 1:A:150:ARG:HB2  | 1.71                     | 0.56              |
| 1:C:83:ALA:HA    | 1:H:111:ARG:HH12 | 1.69                     | 0.56              |
| 1:L:112:ARG:HH11 | 1:L:211:LEU:HD21 | 1.69                     | 0.56              |
| 1:J:169:ARG:HG3  | 1:J:234:VAL:HG11 | 1.87                     | 0.56              |
| 1:K:245:LEU:O    | 1:K:249:ILE:HG12 | 2.05                     | 0.56              |
| 1:K:253:SER:C    | 1:K:255:ARG:H    | 2.09                     | 0.56              |
| 1:A:214:HIS:HD2  | 1:A:258:SER:OG   | 1.88                     | 0.56              |
| 1:C:125:ASN:O    | 1:C:138:MET:HB3  | 2.06                     | 0.56              |
| 1:J:161:LYS:HG3  | 2:J:293:HOH:O    | 2.06                     | 0.56              |
| 1:J:37:GLU:HB2   | 2:J:298:HOH:O    | 2.05                     | 0.56              |
| 1:M:188:THR:O    | 1:M:191:GLU:HB2  | 2.05                     | 0.56              |
| 1:M:244:HIS:O    | 1:M:248:GLU:CG   | 2.54                     | 0.56              |
| 1:K:124:PHE:CD2  | 1:K:179:LEU:HG   | 2.41                     | 0.56              |
| 1:A:244:HIS:O    | 1:A:248:GLU:HG3  | 2.06                     | 0.56              |
| 1:G:122:ALA:O    | 1:G:123:ASP:C    | 2.44                     | 0.55              |
| 1:A:156:ARG:NH1  | 1:D:153:GLU:O    | 2.39                     | 0.55              |
| 1:F:265:ASN:HD22 | 1:F:268:LEU:HD12 | 1.71                     | 0.55              |
| 1:I:169:ARG:HD2  | 1:I:234:VAL:HG12 | 1.89                     | 0.55              |
| 1:L:97:HIS:HE1   | 1:L:119:ASP:HB2  | 1.70                     | 0.55              |
| 1:M:31:ARG:NH1   | 1:M:31:ARG:HB3   | 2.20                     | 0.55              |
| 1:A:169:ARG:HA   | 1:E:290:ILE:CG2  | 2.36                     | 0.55              |
| 1:J:7:VAL:HG13   | 1:J:92:VAL:HG22  | 1.88                     | 0.55              |
| 1:C:129:THR:O    | 1:C:130:SER:CB   | 2.53                     | 0.55              |
| 1:L:214:HIS:HD2  | 1:L:258:SER:OG   | 1.88                     | 0.55              |
| 1:F:169:ARG:NH1  | 1:F:234:VAL:O    | 2.40                     | 0.55              |
| 1:L:124:PHE:HD1  | 1:L:140:LEU:HD23 | 1.71                     | 0.55              |
| 1:C:199:ARG:O    | 1:C:203:GLU:HG3  | 2.05                     | 0.55              |
| 1:L:13:LEU:HB2   | 1:L:70:ILE:HD11  | 1.88                     | 0.55              |
| 1:I:25:SER:HB3   | 1:M:22:MET:HE3   | 1.87                     | 0.55              |
| 1:M:259:LEU:HD13 | 1:M:285:LEU:HD23 | 1.87                     | 0.55              |
| 1:G:128:GLU:N    | 1:G:128:GLU:OE1  | 2.29                     | 0.55              |
| 1:K:290:ILE:H    | 1:K:290:ILE:HD12 | 1.71                     | 0.55              |
| 1:F:91:ILE:HG23  | 1:F:259:LEU:HD23 | 1.89                     | 0.55              |
| 1:J:117:TRP:CD2  | 1:J:140:LEU:HD22 | 2.42                     | 0.55              |
| 1:K:124:PHE:CD1  | 1:K:140:LEU:HG   | 2.42                     | 0.55              |
| 1:I:228:PRO:HD3  | 1:I:273:ARG:HH21 | 1.71                     | 0.55              |
| 1:K:244:HIS:O    | 1:K:248:GLU:HG3  | 2.07                     | 0.55              |
| 1:M:125:ASN:O    | 1:M:138:MET:HG2  | 2.06                     | 0.55              |
| 1:M:225:THR:HG23 | 1:M:226:LEU:N    | 2.21                     | 0.55              |
| 1:I:119:ASP:HB3  | 1:I:121:HIS:O    | 2.05                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:169:ARG:NH2  | 1:D:221:VAL:O    | 2.40                     | 0.55              |
| 1:D:169:ARG:NH2  | 1:D:237:GLY:HA3  | 2.22                     | 0.55              |
| 1:G:145:GLY:HA2  | 1:G:156:ARG:CD   | 2.25                     | 0.55              |
| 1:G:145:GLY:CA   | 1:G:156:ARG:HD3  | 2.24                     | 0.55              |
| 1:C:169:ARG:HD2  | 1:C:234:VAL:O    | 2.06                     | 0.55              |
| 1:C:169:ARG:HH22 | 1:C:221:VAL:C    | 2.09                     | 0.55              |
| 1:M:197:VAL:HG21 | 1:M:242:GLU:HB3  | 1.89                     | 0.55              |
| 1:L:248:GLU:HA   | 2:L:294:HOH:O    | 2.06                     | 0.55              |
| 1:D:112:ARG:NH1  | 1:D:211:LEU:HD21 | 2.21                     | 0.55              |
| 1:I:98:SER:OG    | 1:I:136:HIS:HB3  | 2.07                     | 0.55              |
| 1:A:11:MET:HE3   | 1:A:98:SER:HB2   | 1.89                     | 0.55              |
| 1:L:66:TYR:O     | 1:L:68:GLU:N     | 2.40                     | 0.55              |
| 1:I:127:PRO:HD2  | 1:I:128:GLU:OE1  | 2.06                     | 0.55              |
| 1:G:94:GLY:HA3   | 1:G:99:LEU:HD21  | 1.88                     | 0.55              |
| 1:M:13:LEU:N     | 1:M:96:ASP:OD2   | 2.36                     | 0.55              |
| 1:L:188:THR:O    | 1:L:192:VAL:HG23 | 2.07                     | 0.55              |
| 1:K:159:ASP:O    | 1:K:162:ASP:N    | 2.40                     | 0.55              |
| 1:K:124:PHE:CD1  | 1:K:141:ALA:N    | 2.75                     | 0.55              |
| 1:K:176:LYS:HB3  | 1:M:291:PHE:CE2  | 2.41                     | 0.55              |
| 1:G:201:ALA:HB1  | 1:G:249:ILE:HG21 | 1.89                     | 0.55              |
| 1:M:150:ARG:HD3  | 1:M:150:ARG:O    | 2.07                     | 0.55              |
| 1:M:109:ARG:CG   | 1:M:109:ARG:HH11 | 2.19                     | 0.55              |
| 1:M:29:TYR:C     | 1:M:31:ARG:N     | 2.60                     | 0.55              |
| 1:I:144:SER:HA   | 1:I:158:VAL:O    | 2.07                     | 0.55              |
| 1:J:129:THR:O    | 1:J:130:SER:CB   | 2.54                     | 0.54              |
| 1:G:169:ARG:HH22 | 1:G:221:VAL:C    | 2.10                     | 0.54              |
| 1:D:96:ASP:HB3   | 1:D:136:HIS:HB3  | 1.89                     | 0.54              |
| 1:H:97:HIS:O     | 1:H:100:SER:HB2  | 2.07                     | 0.54              |
| 1:M:159:ASP:O    | 1:M:162:ASP:HB2  | 2.07                     | 0.54              |
| 1:G:156:ARG:HG2  | 1:G:156:ARG:HH11 | 1.72                     | 0.54              |
| 1:G:26:ALA:HB1   | 1:G:272:ASN:OD1  | 2.07                     | 0.54              |
| 1:D:143:LEU:O    | 1:D:158:VAL:HG12 | 2.07                     | 0.54              |
| 1:H:173:PRO:HA   | 1:H:176:LYS:HG3  | 1.89                     | 0.54              |
| 1:D:189:MET:HA   | 1:D:189:MET:HE3  | 1.90                     | 0.54              |
| 1:K:109:ARG:C    | 1:K:111:ARG:H    | 2.10                     | 0.54              |
| 1:D:192:VAL:HA   | 1:D:200:ILE:HD11 | 1.90                     | 0.54              |
| 1:H:112:ARG:HD3  | 1:H:211:LEU:HD22 | 1.90                     | 0.54              |
| 1:C:148:HIS:HD2  | 1:C:150:ARG:N    | 2.01                     | 0.54              |
| 1:L:3:ARG:CZ     | 1:L:88:VAL:HG23  | 2.38                     | 0.54              |
| 1:I:138:MET:N    | 1:I:139:PRO:CD   | 2.68                     | 0.54              |
| 1:H:119:ASP:OD2  | 1:H:123:ASP:OD2  | 2.25                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:148:HIS:CD2  | 1:I:149:PRO:HD2  | 2.42                     | 0.54              |
| 1:M:4:VAL:CG2    | 1:M:41:TYR:HD1   | 2.20                     | 0.54              |
| 1:M:82:ALA:C     | 1:M:84:LEU:H     | 2.09                     | 0.54              |
| 1:I:91:ILE:HD11  | 1:I:286:LEU:HD21 | 1.89                     | 0.54              |
| 1:L:205:LEU:HD13 | 1:L:253:SER:HB3  | 1.89                     | 0.54              |
| 1:C:30:ALA:CB    | 1:C:279:VAL:HG21 | 2.36                     | 0.54              |
| 1:J:187:TYR:CD1  | 1:J:200:ILE:HD12 | 2.43                     | 0.54              |
| 1:M:247:MET:HB2  | 1:M:284:SER:HB3  | 1.90                     | 0.54              |
| 1:A:99:LEU:C     | 1:A:99:LEU:HD12  | 2.28                     | 0.54              |
| 1:K:112:ARG:HD3  | 1:K:211:LEU:HD21 | 1.90                     | 0.54              |
| 1:J:125:ASN:ND2  | 1:J:175:GLU:CG   | 2.67                     | 0.54              |
| 1:H:11:MET:HE1   | 1:H:98:SER:HB2   | 1.89                     | 0.54              |
| 1:L:126:THR:HG23 | 1:L:178:LEU:HD13 | 1.90                     | 0.54              |
| 1:A:79:GLU:CG    | 1:D:111:ARG:NH2  | 2.70                     | 0.54              |
| 1:J:86:GLU:HG2   | 1:J:109:ARG:NE   | 2.21                     | 0.54              |
| 1:I:261:LEU:HD11 | 1:I:282:ALA:HB2  | 1.90                     | 0.54              |
| 1:L:12:ASP:HB2   | 1:L:20:VAL:HG23  | 1.90                     | 0.54              |
| 1:M:22:MET:HB2   | 1:M:266:PRO:CG   | 2.38                     | 0.54              |
| 1:F:123:ASP:HB3  | 1:F:139:PRO:HD2  | 1.88                     | 0.54              |
| 1:M:22:MET:SD    | 1:M:267:ILE:HD13 | 2.48                     | 0.54              |
| 1:D:117:TRP:HB3  | 1:D:165:LEU:HD23 | 1.91                     | 0.54              |
| 1:D:113:VAL:HG12 | 1:D:212:PRO:HG2  | 1.90                     | 0.54              |
| 1:A:125:ASN:ND2  | 1:A:175:GLU:HG3  | 2.23                     | 0.54              |
| 1:M:129:THR:HB   | 1:M:174:GLY:CA   | 2.25                     | 0.53              |
| 1:A:153:GLU:HA   | 1:D:156:ARG:NH2  | 2.23                     | 0.53              |
| 1:M:124:PHE:CE2  | 1:M:178:LEU:HB3  | 2.41                     | 0.53              |
| 1:L:265:ASN:ND2  | 1:L:268:LEU:HD13 | 2.23                     | 0.53              |
| 1:G:279:VAL:O    | 1:G:283:LEU:HG   | 2.08                     | 0.53              |
| 1:M:117:TRP:O    | 1:M:165:LEU:HD23 | 2.08                     | 0.53              |
| 1:M:122:ALA:HB2  | 1:M:171:LEU:CD2  | 2.38                     | 0.53              |
| 1:L:196:GLY:O    | 1:L:200:ILE:HG13 | 2.08                     | 0.53              |
| 1:K:215:VAL:O    | 1:K:259:LEU:HD12 | 2.07                     | 0.53              |
| 1:K:215:VAL:HB   | 1:K:259:LEU:HD13 | 1.89                     | 0.53              |
| 1:M:226:LEU:HD21 | 1:M:240:TYR:CB   | 2.33                     | 0.53              |
| 1:D:11:MET:HG2   | 1:D:96:ASP:OD2   | 2.08                     | 0.53              |
| 1:L:100:SER:HA   | 1:L:103:SER:OG   | 2.08                     | 0.53              |
| 1:L:189:MET:HA   | 1:L:192:VAL:CG2  | 2.38                     | 0.53              |
| 1:I:25:SER:HB3   | 1:M:22:MET:HE2   | 1.90                     | 0.53              |
| 1:I:35:GLN:OE1   | 1:I:283:LEU:HD11 | 2.08                     | 0.53              |
| 1:F:270:GLU:O    | 1:F:273:ARG:HG2  | 2.08                     | 0.53              |
| 1:E:216:SER:HA   | 1:E:260:ASP:HB2  | 1.90                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:97:HIS:ND1   | 1:K:119:ASP:OD2  | 2.42                     | 0.53              |
| 1:M:124:PHE:O    | 1:M:124:PHE:CD2  | 2.62                     | 0.53              |
| 1:J:122:ALA:O    | 1:J:124:PHE:HB2  | 2.09                     | 0.53              |
| 1:L:145:GLY:HA3  | 1:L:156:ARG:CD   | 2.38                     | 0.53              |
| 1:J:4:VAL:HG22   | 1:J:89:PHE:HB3   | 1.90                     | 0.53              |
| 1:F:177:ARG:HG2  | 1:F:177:ARG:HH11 | 1.74                     | 0.53              |
| 1:C:81:LEU:C     | 1:C:83:ALA:H     | 2.12                     | 0.53              |
| 1:L:33:LEU:HD23  | 1:L:43:VAL:CB    | 2.36                     | 0.53              |
| 1:F:140:LEU:HD11 | 1:F:163:VAL:HG11 | 1.89                     | 0.53              |
| 1:M:148:HIS:HD2  | 1:M:150:ARG:H    | 1.57                     | 0.53              |
| 1:M:94:GLY:HA2   | 1:M:99:LEU:CD2   | 2.39                     | 0.53              |
| 1:H:97:HIS:CE1   | 1:H:218:ASP:HB2  | 2.43                     | 0.53              |
| 1:A:228:PRO:HG2  | 1:A:269:ASP:OD1  | 2.09                     | 0.53              |
| 1:L:64:LEU:HD13  | 1:L:65:ALA:N     | 2.24                     | 0.53              |
| 1:K:277:MET:HA   | 1:K:277:MET:CE   | 2.39                     | 0.53              |
| 1:L:37:GLU:O     | 1:L:40:GLY:N     | 2.35                     | 0.53              |
| 1:I:11:MET:HE2   | 1:I:98:SER:HB2   | 1.88                     | 0.53              |
| 1:I:32:LEU:HD12  | 1:I:279:VAL:HG13 | 1.90                     | 0.53              |
| 1:L:81:LEU:HD13  | 1:L:107:ALA:HB2  | 1.90                     | 0.53              |
| 1:J:117:TRP:HB3  | 1:J:165:LEU:HD23 | 1.90                     | 0.53              |
| 1:I:165:LEU:HD12 | 1:I:186:VAL:HG22 | 1.90                     | 0.53              |
| 1:L:97:HIS:ND1   | 1:L:218:ASP:OD2  | 2.42                     | 0.53              |
| 1:A:31:ARG:HA    | 1:A:34:GLU:OE1   | 2.09                     | 0.53              |
| 1:M:41:TYR:O     | 1:M:43:VAL:HG23  | 2.09                     | 0.53              |
| 1:D:169:ARG:HG3  | 1:D:234:VAL:HG11 | 1.90                     | 0.53              |
| 1:K:270:GLU:HB2  | 1:K:273:ARG:HD3  | 1.89                     | 0.53              |
| 1:K:272:ASN:O    | 1:K:276:GLU:HG3  | 2.09                     | 0.53              |
| 1:J:111:ARG:HD3  | 1:J:112:ARG:H    | 1.74                     | 0.53              |
| 1:H:51:VAL:O     | 1:H:51:VAL:HG12  | 2.09                     | 0.53              |
| 1:A:138:MET:H    | 1:A:139:PRO:CD   | 2.21                     | 0.53              |
| 1:H:156:ARG:HG2  | 1:H:156:ARG:NH1  | 2.23                     | 0.53              |
| 1:D:169:ARG:HD3  | 1:D:235:PRO:O    | 2.09                     | 0.53              |
| 1:M:144:SER:OG   | 1:M:160:PRO:HG3  | 2.09                     | 0.53              |
| 1:M:287:GLY:O    | 1:M:289:ARG:HD3  | 2.08                     | 0.53              |
| 1:K:91:ILE:HA    | 1:K:259:LEU:O    | 2.09                     | 0.52              |
| 1:J:149:PRO:HA   | 1:J:152:THR:OG1  | 2.08                     | 0.52              |
| 1:C:138:MET:N    | 1:C:139:PRO:CD   | 2.72                     | 0.52              |
| 1:G:75:LEU:O     | 1:G:79:GLU:HG3   | 2.09                     | 0.52              |
| 1:F:198:ALA:O    | 1:F:202:GLU:HG2  | 2.08                     | 0.52              |
| 1:I:20:VAL:HG12  | 1:I:265:ASN:HB2  | 1.91                     | 0.52              |
| 1:M:126:THR:C    | 1:M:128:GLU:N    | 2.61                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:97:HIS:ND1   | 1:K:123:ASP:OD2  | 2.42                     | 0.52              |
| 1:D:156:ARG:HH11 | 1:D:156:ARG:HG2  | 1.73                     | 0.52              |
| 1:I:179:LEU:HD23 | 1:I:184:VAL:HB   | 1.91                     | 0.52              |
| 1:D:119:ASP:OD2  | 1:D:218:ASP:OD2  | 2.26                     | 0.52              |
| 1:M:225:THR:CG2  | 1:M:226:LEU:N    | 2.72                     | 0.52              |
| 1:K:243:ALA:O    | 1:K:247:MET:HG2  | 2.10                     | 0.52              |
| 1:M:213:LEU:O    | 1:M:257:GLN:N    | 2.43                     | 0.52              |
| 1:G:12:ASP:HB2   | 1:G:21:ASP:HB3   | 1.92                     | 0.52              |
| 1:M:29:TYR:O     | 1:M:31:ARG:HG3   | 2.09                     | 0.52              |
| 1:J:169:ARG:NH2  | 1:J:237:GLY:HA3  | 2.25                     | 0.52              |
| 1:K:8:GLY:O      | 1:K:48:ASP:HA    | 2.09                     | 0.52              |
| 1:A:111:ARG:CD   | 1:A:112:ARG:H    | 2.18                     | 0.52              |
| 1:J:204:VAL:C    | 1:J:206:LYS:N    | 2.62                     | 0.52              |
| 1:I:13:LEU:HD22  | 1:I:66:TYR:CD1   | 2.45                     | 0.52              |
| 1:K:237:GLY:O    | 1:M:241:ARG:NH1  | 2.42                     | 0.52              |
| 1:E:221:VAL:O    | 1:E:221:VAL:HG22 | 2.08                     | 0.52              |
| 1:E:19:GLY:N     | 1:E:265:ASN:HD21 | 2.08                     | 0.52              |
| 1:H:109:ARG:NH1  | 1:H:109:ARG:CG   | 2.61                     | 0.52              |
| 1:M:153:GLU:CG   | 1:M:154:VAL:H    | 2.18                     | 0.52              |
| 1:F:11:MET:CE    | 1:F:98:SER:HB2   | 2.39                     | 0.52              |
| 1:H:13:LEU:HB2   | 1:H:70:ILE:HD11  | 1.91                     | 0.52              |
| 1:F:214:HIS:CE1  | 1:F:260:ASP:OD2  | 2.62                     | 0.52              |
| 1:C:83:ALA:HB1   | 1:H:111:ARG:NH1  | 2.23                     | 0.52              |
| 1:I:130:SER:OG   | 1:I:132:SER:N    | 2.36                     | 0.52              |
| 1:A:109:ARG:CG   | 1:A:109:ARG:HH11 | 2.21                     | 0.52              |
| 1:L:124:PHE:CD1  | 1:L:140:LEU:HD23 | 2.44                     | 0.52              |
| 1:K:159:ASP:C    | 1:K:161:LYS:N    | 2.63                     | 0.52              |
| 1:I:13:LEU:HD13  | 1:I:70:ILE:HG13  | 1.92                     | 0.52              |
| 1:F:94:GLY:HA3   | 1:F:99:LEU:HD21  | 1.92                     | 0.52              |
| 1:E:259:LEU:HD22 | 1:E:285:LEU:HD23 | 1.91                     | 0.52              |
| 1:M:118:VAL:HG13 | 1:M:166:VAL:HB   | 1.91                     | 0.52              |
| 1:C:81:LEU:C     | 1:C:83:ALA:N     | 2.61                     | 0.52              |
| 1:I:170:SER:O    | 1:I:171:LEU:HD23 | 2.10                     | 0.52              |
| 1:L:190:HIS:HE1  | 1:L:194:ARG:NE   | 2.03                     | 0.52              |
| 1:M:125:ASN:C    | 1:M:138:MET:HG2  | 2.30                     | 0.51              |
| 1:K:109:ARG:O    | 1:K:111:ARG:N    | 2.41                     | 0.51              |
| 1:M:80:ARG:HD2   | 1:M:80:ARG:C     | 2.29                     | 0.51              |
| 1:E:271:ARG:HH22 | 1:F:228:PRO:HB3  | 1.75                     | 0.51              |
| 1:M:169:ARG:NH1  | 1:M:234:VAL:O    | 2.42                     | 0.51              |
| 1:F:20:VAL:HB    | 1:F:95:GLY:HA2   | 1.92                     | 0.51              |
| 1:D:129:THR:HB   | 1:D:174:GLY:HA3  | 1.93                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:130:SER:OG   | 1:J:132:SER:N    | 2.33                     | 0.51              |
| 1:M:20:VAL:O     | 1:M:95:GLY:HA2   | 2.11                     | 0.51              |
| 1:A:156:ARG:CZ   | 1:D:156:ARG:NH2  | 2.74                     | 0.51              |
| 1:D:122:ALA:O    | 1:D:123:ASP:C    | 2.48                     | 0.51              |
| 1:D:22:MET:CE    | 1:J:22:MET:HB3   | 2.40                     | 0.51              |
| 1:K:277:MET:HA   | 1:K:277:MET:HE3  | 1.92                     | 0.51              |
| 1:G:120:ALA:HB2  | 1:G:220:ASP:O    | 2.11                     | 0.51              |
| 1:C:97:HIS:CE1   | 1:C:119:ASP:OD2  | 2.64                     | 0.51              |
| 1:J:119:ASP:OD2  | 1:J:218:ASP:OD2  | 2.29                     | 0.51              |
| 1:D:216:SER:HA   | 1:D:260:ASP:HB2  | 1.92                     | 0.51              |
| 1:J:118:VAL:HG12 | 1:J:221:VAL:HG21 | 1.93                     | 0.51              |
| 1:M:13:LEU:N     | 1:M:13:LEU:HD23  | 2.25                     | 0.51              |
| 1:H:97:HIS:ND1   | 1:H:218:ASP:OD2  | 2.44                     | 0.51              |
| 1:I:20:VAL:HB    | 1:I:95:GLY:HA2   | 1.92                     | 0.51              |
| 1:E:118:VAL:HG12 | 1:E:221:VAL:HG21 | 1.92                     | 0.51              |
| 1:E:26:ALA:HB1   | 1:E:272:ASN:OD1  | 2.11                     | 0.51              |
| 1:I:44:GLU:HG2   | 1:I:46:LEU:HD23  | 1.92                     | 0.51              |
| 1:G:117:TRP:HB3  | 1:G:165:LEU:CD2  | 2.35                     | 0.51              |
| 1:H:119:ASP:HA   | 1:H:218:ASP:HB3  | 1.93                     | 0.51              |
| 1:I:259:LEU:HD21 | 1:I:261:LEU:HD21 | 1.91                     | 0.51              |
| 1:L:169:ARG:NH2  | 1:L:237:GLY:HA2  | 2.25                     | 0.51              |
| 1:I:94:GLY:HA3   | 1:I:99:LEU:CD2   | 2.40                     | 0.51              |
| 1:M:128:GLU:C    | 1:M:130:SER:H    | 2.13                     | 0.51              |
| 1:M:223:ASP:OD2  | 1:M:225:THR:HG22 | 2.11                     | 0.51              |
| 1:A:129:THR:O    | 1:A:130:SER:CB   | 2.59                     | 0.51              |
| 1:K:243:ALA:C    | 1:K:281:LEU:HD21 | 2.31                     | 0.51              |
| 1:E:98:SER:OG    | 1:E:136:HIS:HB3  | 2.11                     | 0.51              |
| 1:A:248:GLU:O    | 1:A:252:GLU:HG3  | 2.11                     | 0.51              |
| 1:I:68:GLU:OE2   | 1:I:150:ARG:NE   | 2.44                     | 0.51              |
| 1:C:4:VAL:HG22   | 1:C:89:PHE:HB3   | 1.92                     | 0.51              |
| 1:A:65:ALA:O     | 1:A:66:TYR:HB2   | 2.09                     | 0.51              |
| 1:M:168:VAL:CG1  | 1:M:168:VAL:O    | 2.58                     | 0.51              |
| 1:K:190:HIS:HD2  | 1:M:248:GLU:OE1  | 1.94                     | 0.51              |
| 1:A:148:HIS:CD2  | 1:A:150:ARG:HB2  | 2.46                     | 0.51              |
| 1:I:126:THR:HG23 | 1:I:178:LEU:CD1  | 2.41                     | 0.51              |
| 1:G:226:LEU:HD11 | 1:G:277:MET:SD   | 2.50                     | 0.51              |
| 1:M:203:GLU:O    | 1:M:206:LYS:HB3  | 2.11                     | 0.51              |
| 1:G:22:MET:SD    | 1:G:267:ILE:HD11 | 2.50                     | 0.51              |
| 1:E:4:VAL:HG12   | 1:E:43:VAL:HG13  | 1.91                     | 0.50              |
| 1:C:169:ARG:NH2  | 1:C:221:VAL:O    | 2.44                     | 0.50              |
| 1:I:109:ARG:HH11 | 1:I:109:ARG:CG   | 2.22                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:169:ARG:HB3  | 1:M:189:MET:HG2  | 1.93                     | 0.50              |
| 1:E:11:MET:HE1   | 1:E:98:SER:HB2   | 1.92                     | 0.50              |
| 1:C:111:ARG:CD   | 1:C:112:ARG:H    | 2.23                     | 0.50              |
| 1:C:83:ALA:HB1   | 1:H:111:ARG:NH2  | 2.25                     | 0.50              |
| 1:K:97:HIS:CD2   | 1:K:262:VAL:HG21 | 2.45                     | 0.50              |
| 1:D:43:VAL:CG1   | 1:D:44:GLU:N     | 2.73                     | 0.50              |
| 1:A:72:ALA:O     | 1:A:76:VAL:HG23  | 2.11                     | 0.50              |
| 1:M:129:THR:O    | 1:M:130:SER:HB2  | 2.12                     | 0.50              |
| 1:F:122:ALA:O    | 1:F:123:ASP:C    | 2.49                     | 0.50              |
| 1:A:97:HIS:ND1   | 1:A:123:ASP:OD2  | 2.44                     | 0.50              |
| 1:E:104:VAL:O    | 1:E:108:ALA:HB2  | 2.12                     | 0.50              |
| 1:H:26:ALA:HB1   | 1:H:272:ASN:OD1  | 2.12                     | 0.50              |
| 1:G:33:LEU:HG    | 1:G:43:VAL:HG11  | 1.94                     | 0.50              |
| 1:E:158:VAL:HG22 | 1:E:159:ASP:N    | 2.27                     | 0.50              |
| 1:H:32:LEU:HA    | 1:H:279:VAL:HG13 | 1.93                     | 0.50              |
| 1:J:187:TYR:OH   | 1:J:203:GLU:HG2  | 2.11                     | 0.50              |
| 1:C:11:MET:CE    | 1:C:98:SER:HB2   | 2.42                     | 0.50              |
| 1:L:118:VAL:HB   | 1:L:217:LEU:HD12 | 1.93                     | 0.50              |
| 1:M:249:ILE:O    | 1:M:252:GLU:HB2  | 2.11                     | 0.50              |
| 1:H:90:PRO:HD2   | 1:H:257:GLN:O    | 2.10                     | 0.50              |
| 1:A:79:GLU:CG    | 1:D:111:ARG:HH22 | 2.24                     | 0.50              |
| 1:E:97:HIS:ND1   | 1:E:119:ASP:OD2  | 2.44                     | 0.50              |
| 1:M:122:ALA:HB2  | 1:M:171:LEU:HD21 | 1.93                     | 0.50              |
| 1:F:142:VAL:O    | 1:F:145:GLY:N    | 2.42                     | 0.50              |
| 1:H:99:LEU:HD12  | 1:H:100:SER:N    | 2.27                     | 0.50              |
| 1:F:169:ARG:NH2  | 1:F:221:VAL:O    | 2.44                     | 0.50              |
| 1:L:98:SER:OG    | 1:L:136:HIS:HB3  | 2.11                     | 0.50              |
| 1:M:30:ALA:HB1   | 1:M:276:GLU:HA   | 1.92                     | 0.50              |
| 1:L:148:HIS:CD2  | 1:L:150:ARG:HB2  | 2.45                     | 0.50              |
| 1:K:115:VAL:HB   | 1:K:163:VAL:HG22 | 1.94                     | 0.50              |
| 1:I:212:PRO:HA   | 1:I:255:ARG:O    | 2.12                     | 0.50              |
| 1:C:118:VAL:HG12 | 1:C:221:VAL:HG21 | 1.94                     | 0.50              |
| 1:M:188:THR:O    | 1:M:192:VAL:HG23 | 2.11                     | 0.50              |
| 1:H:111:ARG:NE   | 1:H:112:ARG:N    | 2.59                     | 0.50              |
| 1:L:177:ARG:O    | 1:L:179:LEU:N    | 2.44                     | 0.50              |
| 1:H:153:GLU:HG3  | 1:H:154:VAL:HG13 | 1.92                     | 0.50              |
| 1:E:169:ARG:NH1  | 1:E:234:VAL:O    | 2.45                     | 0.50              |
| 1:H:115:VAL:HB   | 1:H:163:VAL:HG22 | 1.94                     | 0.50              |
| 1:H:82:ALA:HA    | 1:H:109:ARG:NH1  | 2.20                     | 0.50              |
| 1:I:89:PHE:CE2   | 1:I:286:LEU:HD11 | 2.46                     | 0.50              |
| 1:D:97:HIS:ND1   | 1:D:119:ASP:OD2  | 2.45                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:228:PRO:HG3  | 1:E:270:GLU:HG3  | 1.93                     | 0.50              |
| 1:I:27:LEU:HD13  | 1:I:93:LEU:HD22  | 1.93                     | 0.50              |
| 1:F:144:SER:HB3  | 1:F:160:PRO:HG3  | 1.94                     | 0.50              |
| 1:M:173:PRO:HG2  | 2:M:293:HOH:O    | 2.11                     | 0.50              |
| 1:I:100:SER:HA   | 1:I:103:SER:OG   | 2.12                     | 0.50              |
| 1:I:168:VAL:O    | 1:I:188:THR:HA   | 2.12                     | 0.50              |
| 1:G:97:HIS:NE2   | 1:G:117:TRP:CZ2  | 2.80                     | 0.49              |
| 1:J:143:LEU:O    | 1:J:158:VAL:HG12 | 2.11                     | 0.49              |
| 1:C:221:VAL:HG22 | 1:C:221:VAL:O    | 2.12                     | 0.49              |
| 1:M:97:HIS:ND1   | 1:M:119:ASP:OD2  | 2.45                     | 0.49              |
| 1:A:22:MET:CE    | 1:H:25:SER:HB2   | 2.42                     | 0.49              |
| 1:D:259:LEU:HD13 | 1:D:285:LEU:CD2  | 2.41                     | 0.49              |
| 1:K:124:PHE:CE1  | 1:K:140:LEU:HG   | 2.47                     | 0.49              |
| 1:C:11:MET:HE1   | 1:C:98:SER:HB2   | 1.94                     | 0.49              |
| 1:E:12:ASP:HB2   | 1:E:21:ASP:HB3   | 1.93                     | 0.49              |
| 1:L:109:ARG:NH1  | 1:L:109:ARG:CG   | 2.65                     | 0.49              |
| 1:F:138:MET:N    | 1:F:139:PRO:HD3  | 2.26                     | 0.49              |
| 1:H:119:ASP:OD1  | 1:H:120:ALA:N    | 2.44                     | 0.49              |
| 1:I:32:LEU:CD1   | 1:I:279:VAL:HG13 | 2.42                     | 0.49              |
| 1:J:89:PHE:HD2   | 1:J:91:ILE:HD12  | 1.78                     | 0.49              |
| 1:I:213:LEU:HD11 | 1:I:255:ARG:NH1  | 2.26                     | 0.49              |
| 1:K:128:GLU:CD   | 1:K:128:GLU:H    | 2.15                     | 0.49              |
| 1:D:33:LEU:HD11  | 1:D:45:ASP:HB2   | 1.94                     | 0.49              |
| 1:I:51:VAL:CG1   | 1:I:52:SER:N     | 2.75                     | 0.49              |
| 1:F:122:ALA:O    | 1:F:124:PHE:HB2  | 2.11                     | 0.49              |
| 1:J:124:PHE:HD1  | 1:J:140:LEU:HB3  | 1.78                     | 0.49              |
| 1:H:135:VAL:O    | 1:H:139:PRO:HD3  | 2.12                     | 0.49              |
| 1:I:11:MET:HE3   | 1:I:70:ILE:HG12  | 1.93                     | 0.49              |
| 1:G:195:LEU:HB2  | 1:G:200:ILE:HD11 | 1.94                     | 0.49              |
| 1:G:99:LEU:HD12  | 1:G:100:SER:N    | 2.26                     | 0.49              |
| 1:E:169:ARG:HH11 | 1:E:234:VAL:HB   | 1.76                     | 0.49              |
| 1:F:19:GLY:N     | 2:F:302:HOH:O    | 2.45                     | 0.49              |
| 1:F:188:THR:HG21 | 1:H:291:PHE:HB2  | 1.94                     | 0.49              |
| 1:A:111:ARG:NH1  | 1:D:83:ALA:HB2   | 2.19                     | 0.49              |
| 1:E:127:PRO:N    | 1:E:138:MET:HE1  | 2.27                     | 0.49              |
| 1:G:119:ASP:HA   | 1:G:218:ASP:HB3  | 1.93                     | 0.49              |
| 1:G:130:SER:OG   | 1:G:132:SER:N    | 2.46                     | 0.49              |
| 1:F:192:VAL:HA   | 1:F:200:ILE:HD12 | 1.95                     | 0.49              |
| 1:I:11:MET:HE1   | 1:I:98:SER:HB2   | 1.91                     | 0.49              |
| 1:M:41:TYR:CD2   | 1:M:41:TYR:N     | 2.79                     | 0.49              |
| 1:E:198:ALA:O    | 1:E:202:GLU:HG2  | 2.13                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:112:ARG:HD3  | 1:E:211:LEU:HD21 | 1.93                     | 0.49              |
| 1:L:112:ARG:HD3  | 1:L:211:LEU:HD22 | 1.94                     | 0.49              |
| 1:J:152:THR:O    | 1:J:156:ARG:HB2  | 2.11                     | 0.49              |
| 1:F:138:MET:N    | 1:F:139:PRO:CD   | 2.75                     | 0.49              |
| 1:L:186:VAL:O    | 1:L:186:VAL:HG12 | 2.11                     | 0.49              |
| 1:E:79:GLU:HB3   | 2:E:303:HOH:O    | 2.13                     | 0.49              |
| 1:J:207:HIS:O    | 1:J:207:HIS:CD2  | 2.66                     | 0.49              |
| 1:C:83:ALA:CB    | 1:H:111:ARG:NH1  | 2.76                     | 0.49              |
| 1:D:43:VAL:HG12  | 1:D:44:GLU:H     | 1.77                     | 0.49              |
| 1:J:169:ARG:NH2  | 1:J:221:VAL:O    | 2.46                     | 0.49              |
| 1:G:100:SER:HA   | 1:G:103:SER:OG   | 2.13                     | 0.49              |
| 1:E:88:VAL:HG12  | 1:E:88:VAL:O     | 2.12                     | 0.49              |
| 1:C:86:GLU:OE2   | 1:C:109:ARG:HD3  | 2.12                     | 0.49              |
| 1:J:99:LEU:HD12  | 1:J:100:SER:N    | 2.27                     | 0.49              |
| 1:D:223:ASP:OD2  | 1:D:225:THR:CG2  | 2.61                     | 0.49              |
| 1:C:11:MET:HG2   | 1:C:96:ASP:OD2   | 2.12                     | 0.49              |
| 1:K:279:VAL:O    | 1:K:283:LEU:HG   | 2.12                     | 0.49              |
| 1:E:156:ARG:HG2  | 1:E:156:ARG:NH1  | 2.28                     | 0.49              |
| 1:K:158:VAL:HG22 | 1:K:159:ASP:N    | 2.27                     | 0.49              |
| 1:G:173:PRO:HA   | 1:G:176:LYS:HG3  | 1.95                     | 0.49              |
| 1:F:66:TYR:HB3   | 1:F:69:GLU:HB2   | 1.95                     | 0.49              |
| 1:C:169:ARG:HD2  | 1:C:234:VAL:HB   | 1.93                     | 0.49              |
| 1:L:201:ALA:CB   | 1:L:249:ILE:HG21 | 2.42                     | 0.49              |
| 1:F:115:VAL:CG2  | 1:F:158:VAL:HG21 | 2.42                     | 0.49              |
| 1:L:200:ILE:HA   | 1:L:203:GLU:HB2  | 1.95                     | 0.49              |
| 1:K:270:GLU:O    | 1:K:273:ARG:HG2  | 2.13                     | 0.49              |
| 1:J:226:LEU:HD21 | 1:J:240:TYR:HB2  | 1.94                     | 0.49              |
| 1:K:75:LEU:O     | 1:K:79:GLU:HB2   | 2.13                     | 0.49              |
| 1:K:137:GLY:HA3  | 2:K:293:HOH:O    | 2.13                     | 0.49              |
| 1:M:19:GLY:N     | 1:M:265:ASN:HD21 | 2.11                     | 0.48              |
| 1:L:117:TRP:HB3  | 1:L:165:LEU:HD23 | 1.95                     | 0.48              |
| 1:K:124:PHE:CE1  | 1:K:141:ALA:HA   | 2.48                     | 0.48              |
| 1:K:264:VAL:CG2  | 1:K:278:LEU:HD22 | 2.43                     | 0.48              |
| 1:K:4:VAL:HG12   | 1:K:43:VAL:HG13  | 1.95                     | 0.48              |
| 1:D:199:ARG:O    | 1:D:203:GLU:HG3  | 2.13                     | 0.48              |
| 1:E:67:LEU:HD23  | 1:E:67:LEU:C     | 2.33                     | 0.48              |
| 1:M:135:VAL:O    | 1:M:139:PRO:HD3  | 2.14                     | 0.48              |
| 1:L:25:SER:O     | 1:L:29:TYR:CD2   | 2.52                     | 0.48              |
| 1:C:226:LEU:HD21 | 1:C:240:TYR:HB2  | 1.95                     | 0.48              |
| 1:I:33:LEU:HD11  | 1:I:45:ASP:HB2   | 1.95                     | 0.48              |
| 1:A:171:LEU:HB2  | 1:A:176:LYS:HE2  | 1.95                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:164:VAL:HG22 | 1:G:185:ARG:HB3  | 1.95                     | 0.48              |
| 1:J:260:ASP:O    | 1:J:261:LEU:HD23 | 2.13                     | 0.48              |
| 1:C:169:ARG:HG3  | 1:C:234:VAL:HG11 | 1.94                     | 0.48              |
| 1:D:97:HIS:ND1   | 1:D:123:ASP:OD2  | 2.46                     | 0.48              |
| 1:E:34:GLU:CD    | 1:E:34:GLU:H     | 2.16                     | 0.48              |
| 1:K:175:GLU:O    | 1:K:176:LYS:C    | 2.52                     | 0.48              |
| 1:K:169:ARG:NH2  | 1:K:221:VAL:O    | 2.46                     | 0.48              |
| 1:H:214:HIS:CD2  | 1:H:258:SER:OG   | 2.66                     | 0.48              |
| 1:A:30:ALA:HB3   | 1:A:279:VAL:HG21 | 1.95                     | 0.48              |
| 1:D:198:ALA:O    | 1:D:202:GLU:HG2  | 2.13                     | 0.48              |
| 1:F:112:ARG:NE   | 1:F:211:LEU:HD21 | 2.28                     | 0.48              |
| 1:K:119:ASP:OD2  | 1:K:218:ASP:OD2  | 2.30                     | 0.48              |
| 1:G:119:ASP:OD2  | 1:G:123:ASP:OD2  | 2.32                     | 0.48              |
| 1:M:222:LEU:HD13 | 1:M:277:MET:HE2  | 1.95                     | 0.48              |
| 1:D:100:SER:HA   | 1:D:103:SER:OG   | 2.12                     | 0.48              |
| 1:K:148:HIS:CD2  | 1:K:150:ARG:HB2  | 2.48                     | 0.48              |
| 1:K:159:ASP:HB3  | 1:K:162:ASP:CG   | 2.33                     | 0.48              |
| 1:A:214:HIS:HE1  | 1:A:260:ASP:OD2  | 1.96                     | 0.48              |
| 1:K:185:ARG:CZ   | 1:K:207:HIS:ND1  | 2.76                     | 0.48              |
| 1:L:213:LEU:O    | 1:L:257:GLN:HG3  | 2.13                     | 0.48              |
| 1:C:33:LEU:HD21  | 1:C:45:ASP:HB2   | 1.95                     | 0.48              |
| 1:A:97:HIS:NE2   | 1:A:117:TRP:CZ2  | 2.81                     | 0.48              |
| 1:C:97:HIS:CD2   | 1:C:262:VAL:HG21 | 2.48                     | 0.48              |
| 1:A:86:GLU:OE1   | 1:D:86:GLU:N     | 2.47                     | 0.48              |
| 1:E:271:ARG:NH2  | 1:F:228:PRO:HB3  | 2.28                     | 0.48              |
| 1:F:264:VAL:CG2  | 1:F:278:LEU:HD22 | 2.43                     | 0.48              |
| 1:F:119:ASP:HB3  | 1:F:121:HIS:O    | 2.13                     | 0.48              |
| 1:D:71:ARG:HD3   | 2:D:295:HOH:O    | 2.12                     | 0.48              |
| 1:G:99:LEU:HD12  | 1:G:99:LEU:C     | 2.34                     | 0.48              |
| 1:M:46:LEU:N     | 1:M:46:LEU:HD23  | 2.28                     | 0.48              |
| 1:J:246:LEU:HG   | 1:J:247:MET:HE1  | 1.96                     | 0.48              |
| 1:C:97:HIS:ND1   | 1:C:119:ASP:OD2  | 2.46                     | 0.48              |
| 1:M:167:GLY:O    | 1:M:168:VAL:C    | 2.51                     | 0.48              |
| 1:I:115:VAL:HB   | 1:I:163:VAL:HG22 | 1.95                     | 0.48              |
| 1:A:169:ARG:HG3  | 1:A:234:VAL:CG1  | 2.44                     | 0.48              |
| 1:J:81:LEU:O     | 1:J:84:LEU:HD12  | 2.13                     | 0.48              |
| 1:E:279:VAL:O    | 1:E:283:LEU:HG   | 2.13                     | 0.48              |
| 1:L:222:LEU:HD13 | 1:L:277:MET:HG2  | 1.95                     | 0.48              |
| 1:E:214:HIS:CD2  | 1:E:258:SER:OG   | 2.66                     | 0.48              |
| 1:K:84:LEU:O     | 1:K:109:ARG:NH2  | 2.47                     | 0.48              |
| 1:K:97:HIS:CE1   | 1:K:119:ASP:OD2  | 2.67                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:225:THR:O    | 1:D:273:ARG:NH2  | 2.46                     | 0.48              |
| 1:D:130:SER:HG   | 1:D:132:SER:N    | 2.11                     | 0.48              |
| 1:F:221:VAL:HG22 | 1:F:221:VAL:O    | 2.14                     | 0.48              |
| 1:K:161:LYS:HA   | 2:K:294:HOH:O    | 2.14                     | 0.48              |
| 1:K:29:TYR:C     | 1:K:31:ARG:H     | 2.17                     | 0.48              |
| 1:J:33:LEU:HD11  | 1:J:45:ASP:HB2   | 1.96                     | 0.48              |
| 1:C:275:ALA:O    | 1:C:279:VAL:HG23 | 2.13                     | 0.48              |
| 1:L:116:VAL:CG1  | 1:L:204:VAL:HG11 | 2.44                     | 0.48              |
| 1:E:117:TRP:CE3  | 1:E:140:LEU:HD13 | 2.48                     | 0.48              |
| 1:M:70:ILE:HG21  | 1:M:135:VAL:HG11 | 1.95                     | 0.48              |
| 1:J:32:LEU:HA    | 1:J:279:VAL:HG13 | 1.95                     | 0.48              |
| 1:H:169:ARG:HH22 | 1:H:221:VAL:C    | 2.16                     | 0.48              |
| 1:K:32:LEU:CD1   | 1:K:279:VAL:HG13 | 2.43                     | 0.48              |
| 1:H:177:ARG:NH1  | 2:H:304:HOH:O    | 2.44                     | 0.48              |
| 1:I:78:LYS:O     | 1:I:78:LYS:HG2   | 2.13                     | 0.48              |
| 1:I:119:ASP:C    | 1:I:221:VAL:HG23 | 2.34                     | 0.48              |
| 1:J:138:MET:H    | 1:J:139:PRO:CD   | 2.26                     | 0.48              |
| 1:M:100:SER:HA   | 1:M:103:SER:OG   | 2.14                     | 0.48              |
| 1:H:11:MET:HE2   | 1:H:96:ASP:HB2   | 1.95                     | 0.48              |
| 1:D:214:HIS:HD2  | 1:D:258:SER:CB   | 2.26                     | 0.48              |
| 1:E:109:ARG:HH11 | 1:E:109:ARG:CG   | 2.27                     | 0.48              |
| 1:A:156:ARG:CZ   | 1:D:153:GLU:HA   | 2.44                     | 0.47              |
| 1:L:153:GLU:HG2  | 1:L:154:VAL:N    | 2.29                     | 0.47              |
| 1:I:215:VAL:O    | 1:I:259:LEU:HD12 | 2.14                     | 0.47              |
| 1:A:200:ILE:O    | 1:A:204:VAL:HG23 | 2.14                     | 0.47              |
| 1:M:151:LEU:HD22 | 1:M:155:PHE:CD2  | 2.49                     | 0.47              |
| 1:K:8:GLY:HA2    | 1:K:93:LEU:HB2   | 1.95                     | 0.47              |
| 1:J:198:ALA:O    | 1:J:202:GLU:HG2  | 2.14                     | 0.47              |
| 1:G:51:VAL:O     | 1:G:51:VAL:HG12  | 2.12                     | 0.47              |
| 1:L:112:ARG:HD3  | 1:L:211:LEU:HD21 | 1.97                     | 0.47              |
| 1:L:125:ASN:N    | 2:L:301:HOH:O    | 2.47                     | 0.47              |
| 1:I:97:HIS:ND1   | 1:I:123:ASP:OD2  | 2.47                     | 0.47              |
| 1:D:214:HIS:HE1  | 1:D:260:ASP:OD2  | 1.97                     | 0.47              |
| 1:K:221:VAL:HG22 | 1:K:238:LEU:HD12 | 1.96                     | 0.47              |
| 1:K:30:ALA:C     | 1:K:31:ARG:HG2   | 2.34                     | 0.47              |
| 1:K:259:LEU:HD12 | 1:K:260:ASP:H    | 1.79                     | 0.47              |
| 1:J:149:PRO:O    | 1:J:153:GLU:HB3  | 2.13                     | 0.47              |
| 1:F:20:VAL:HB    | 1:F:95:GLY:CA    | 2.45                     | 0.47              |
| 1:J:66:TYR:C     | 1:J:70:ILE:HD13  | 2.34                     | 0.47              |
| 1:L:145:GLY:N    | 1:L:156:ARG:HG3  | 2.30                     | 0.47              |
| 1:I:214:HIS:CE1  | 1:I:260:ASP:OD2  | 2.67                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:92:VAL:HG21  | 1:I:103:SER:HB3  | 1.97                     | 0.47              |
| 1:K:152:THR:O    | 1:K:156:ARG:HB3  | 2.15                     | 0.47              |
| 1:G:146:LEU:CD2  | 1:G:146:LEU:N    | 2.70                     | 0.47              |
| 1:L:149:PRO:O    | 1:L:153:GLU:CB   | 2.62                     | 0.47              |
| 1:A:11:MET:HE1   | 1:A:98:SER:HB2   | 1.96                     | 0.47              |
| 1:I:92:VAL:HG11  | 1:I:99:LEU:HD13  | 1.95                     | 0.47              |
| 1:L:13:LEU:HD23  | 1:L:66:TYR:CD1   | 2.49                     | 0.47              |
| 1:C:20:VAL:HB    | 1:C:95:GLY:HA2   | 1.96                     | 0.47              |
| 1:M:116:VAL:HB   | 1:M:215:VAL:HG22 | 1.96                     | 0.47              |
| 1:M:97:HIS:CD2   | 1:M:262:VAL:HG21 | 2.50                     | 0.47              |
| 1:D:11:MET:HE3   | 1:D:98:SER:HB2   | 1.94                     | 0.47              |
| 1:D:225:THR:CG2  | 1:D:226:LEU:N    | 2.78                     | 0.47              |
| 1:K:78:LYS:O     | 1:K:106:GLY:HA3  | 2.14                     | 0.47              |
| 1:F:228:PRO:O    | 1:F:230:VAL:N    | 2.41                     | 0.47              |
| 1:I:229:GLY:O    | 1:I:274:THR:HG21 | 2.14                     | 0.47              |
| 1:I:67:LEU:HD21  | 1:I:151:LEU:HD21 | 1.96                     | 0.47              |
| 1:G:86:GLU:OE2   | 1:G:109:ARG:HD3  | 2.14                     | 0.47              |
| 1:K:265:ASN:C    | 1:K:265:ASN:OD1  | 2.53                     | 0.47              |
| 1:I:9:VAL:HG21   | 1:I:77:LEU:HD22  | 1.97                     | 0.47              |
| 1:K:33:LEU:HD23  | 1:K:43:VAL:CG1   | 2.44                     | 0.47              |
| 1:J:2:GLU:HG2    | 2:J:303:HOH:O    | 2.15                     | 0.47              |
| 1:L:125:ASN:HA   | 1:L:125:ASN:HD22 | 1.53                     | 0.47              |
| 1:J:156:ARG:CG   | 1:J:156:ARG:NH1  | 2.73                     | 0.47              |
| 1:L:214:HIS:CD2  | 1:L:258:SER:OG   | 2.68                     | 0.47              |
| 1:K:201:ALA:O    | 1:K:204:VAL:HB   | 2.14                     | 0.47              |
| 1:A:140:LEU:HD21 | 1:A:163:VAL:HG11 | 1.95                     | 0.47              |
| 1:E:36:LEU:HD22  | 1:E:286:LEU:HD23 | 1.97                     | 0.47              |
| 1:H:259:LEU:HD13 | 1:H:285:LEU:CD2  | 2.40                     | 0.47              |
| 1:J:124:PHE:HD2  | 1:J:124:PHE:O    | 1.97                     | 0.47              |
| 1:F:222:LEU:O    | 1:F:223:ASP:C    | 2.53                     | 0.47              |
| 1:D:169:ARG:HH22 | 1:D:221:VAL:C    | 2.18                     | 0.47              |
| 1:H:226:LEU:HD21 | 1:H:240:TYR:HB2  | 1.97                     | 0.47              |
| 1:J:214:HIS:HD2  | 1:J:258:SER:OG   | 1.98                     | 0.47              |
| 1:E:20:VAL:HG11  | 1:E:263:GLU:HA   | 1.97                     | 0.47              |
| 1:L:227:ALA:HB1  | 1:L:274:THR:HG23 | 1.97                     | 0.47              |
| 1:E:31:ARG:O     | 1:E:35:GLN:HG3   | 2.15                     | 0.47              |
| 1:M:32:LEU:HB2   | 1:M:279:VAL:HG22 | 1.97                     | 0.47              |
| 1:G:42:THR:HG23  | 2:G:294:HOH:O    | 2.13                     | 0.47              |
| 1:G:214:HIS:HE1  | 1:G:260:ASP:OD2  | 1.97                     | 0.47              |
| 1:K:92:VAL:HG23  | 1:K:260:ASP:HA   | 1.97                     | 0.47              |
| 1:M:22:MET:O     | 1:M:23:GLY:C     | 2.52                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:259:LEU:HD13 | 1:A:285:LEU:CD2  | 2.44                     | 0.47              |
| 1:K:290:ILE:N    | 1:K:290:ILE:HD12 | 2.30                     | 0.47              |
| 1:A:170:SER:O    | 1:A:171:LEU:HD23 | 2.14                     | 0.47              |
| 1:D:2:GLU:HB2    | 2:D:293:HOH:O    | 2.14                     | 0.47              |
| 1:C:76:VAL:HA    | 1:H:86:GLU:HG3   | 1.96                     | 0.47              |
| 1:I:77:LEU:C     | 1:I:79:GLU:N     | 2.68                     | 0.47              |
| 1:M:169:ARG:HD2  | 1:M:234:VAL:HB   | 1.97                     | 0.47              |
| 1:M:9:VAL:O      | 1:M:11:MET:N     | 2.47                     | 0.46              |
| 1:M:145:GLY:HA2  | 1:M:156:ARG:CD   | 2.45                     | 0.46              |
| 1:G:218:ASP:CG   | 1:G:263:GLU:HG3  | 2.35                     | 0.46              |
| 1:J:187:TYR:CE1  | 1:J:200:ILE:HD12 | 2.50                     | 0.46              |
| 1:E:4:VAL:HG22   | 1:E:89:PHE:HB3   | 1.96                     | 0.46              |
| 1:I:179:LEU:CD2  | 1:I:186:VAL:HG21 | 2.44                     | 0.46              |
| 1:K:78:LYS:CA    | 1:K:102:GLY:O    | 2.63                     | 0.46              |
| 1:A:214:HIS:CD2  | 1:A:258:SER:OG   | 2.67                     | 0.46              |
| 1:K:181:GLU:C    | 1:K:183:GLY:H    | 2.18                     | 0.46              |
| 1:K:257:GLN:HG3  | 1:K:258:SER:N    | 2.29                     | 0.46              |
| 1:F:111:ARG:CD   | 1:F:112:ARG:N    | 2.54                     | 0.46              |
| 1:M:79:GLU:HA    | 1:M:82:ALA:HB3   | 1.96                     | 0.46              |
| 1:I:138:MET:H    | 1:I:139:PRO:HD2  | 1.73                     | 0.46              |
| 1:J:124:PHE:O    | 1:J:124:PHE:CD2  | 2.68                     | 0.46              |
| 1:D:97:HIS:O     | 1:D:100:SER:HB2  | 2.15                     | 0.46              |
| 1:M:246:LEU:HB3  | 1:M:247:MET:HE3  | 1.98                     | 0.46              |
| 1:L:129:THR:HG21 | 1:L:174:GLY:HA3  | 1.97                     | 0.46              |
| 1:K:176:LYS:HD3  | 1:M:291:PHE:CD2  | 2.50                     | 0.46              |
| 1:L:13:LEU:HD23  | 1:L:66:TYR:CE1   | 2.50                     | 0.46              |
| 1:D:209:GLN:HA   | 1:D:255:ARG:NH2  | 2.30                     | 0.46              |
| 1:M:12:ASP:OD1   | 1:M:20:VAL:HG23  | 2.15                     | 0.46              |
| 1:M:145:GLY:HA2  | 1:M:156:ARG:HD2  | 1.97                     | 0.46              |
| 1:I:135:VAL:HA   | 1:I:138:MET:SD   | 2.55                     | 0.46              |
| 1:K:77:LEU:O     | 1:K:78:LYS:C     | 2.53                     | 0.46              |
| 1:L:201:ALA:HB1  | 1:L:249:ILE:CG2  | 2.44                     | 0.46              |
| 1:J:4:VAL:HG13   | 1:J:91:ILE:HD13  | 1.96                     | 0.46              |
| 1:E:214:HIS:HD2  | 1:E:258:SER:OG   | 1.98                     | 0.46              |
| 1:H:75:LEU:HA    | 1:H:75:LEU:HD12  | 1.78                     | 0.46              |
| 1:F:69:GLU:N     | 1:F:69:GLU:OE1   | 2.41                     | 0.46              |
| 1:E:129:THR:O    | 1:E:130:SER:HB2  | 2.15                     | 0.46              |
| 1:G:115:VAL:CG2  | 1:G:158:VAL:HG21 | 2.44                     | 0.46              |
| 1:L:163:VAL:HG12 | 1:L:184:VAL:CG1  | 2.46                     | 0.46              |
| 1:I:279:VAL:O    | 1:I:283:LEU:HG   | 2.16                     | 0.46              |
| 1:M:160:PRO:HB2  | 1:M:182:ALA:O    | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:46:LEU:HD13  | 1:G:80:ARG:CZ    | 2.45                     | 0.46              |
| 1:C:76:VAL:HG22  | 1:H:86:GLU:HG3   | 1.98                     | 0.46              |
| 1:A:122:ALA:O    | 1:A:123:ASP:C    | 2.54                     | 0.46              |
| 1:C:97:HIS:O     | 1:C:100:SER:HB2  | 2.15                     | 0.46              |
| 1:K:144:SER:CB   | 1:K:160:PRO:HG3  | 2.41                     | 0.46              |
| 1:H:11:MET:CE    | 1:H:96:ASP:HB2   | 2.45                     | 0.46              |
| 1:D:213:LEU:N    | 1:D:255:ARG:O    | 2.36                     | 0.46              |
| 1:H:64:LEU:HB3   | 1:H:65:ALA:H     | 1.51                     | 0.46              |
| 1:H:138:MET:N    | 1:H:139:PRO:CD   | 2.77                     | 0.46              |
| 1:C:214:HIS:CE1  | 1:C:260:ASP:OD2  | 2.68                     | 0.46              |
| 1:K:32:LEU:HD13  | 1:K:279:VAL:HG13 | 1.97                     | 0.46              |
| 1:C:83:ALA:C     | 1:H:111:ARG:HH22 | 2.19                     | 0.46              |
| 1:K:92:VAL:CG2   | 1:K:260:ASP:OD1  | 2.64                     | 0.46              |
| 1:M:278:LEU:O    | 1:M:279:VAL:C    | 2.54                     | 0.46              |
| 1:H:145:GLY:HA3  | 1:H:156:ARG:HD2  | 1.97                     | 0.46              |
| 1:C:109:ARG:CG   | 1:C:109:ARG:NH1  | 2.55                     | 0.46              |
| 1:C:46:LEU:HD22  | 1:C:80:ARG:NH2   | 2.30                     | 0.46              |
| 1:I:274:THR:O    | 1:I:277:MET:HB2  | 2.16                     | 0.46              |
| 1:D:248:GLU:O    | 1:D:252:GLU:HG3  | 2.15                     | 0.46              |
| 1:C:225:THR:HG22 | 1:C:226:LEU:H    | 1.81                     | 0.46              |
| 1:M:68:GLU:O     | 1:M:72:ALA:HB2   | 2.16                     | 0.46              |
| 1:C:272:ASN:HB2  | 1:K:267:ILE:HA   | 1.98                     | 0.46              |
| 1:J:150:ARG:O    | 1:J:153:GLU:HG2  | 2.14                     | 0.46              |
| 1:K:70:ILE:CD1   | 1:K:135:VAL:HG21 | 2.46                     | 0.46              |
| 1:M:33:LEU:O     | 1:M:34:GLU:C     | 2.55                     | 0.46              |
| 1:J:124:PHE:CD1  | 1:J:140:LEU:HB3  | 2.51                     | 0.46              |
| 1:I:214:HIS:HE1  | 1:I:260:ASP:OD2  | 1.99                     | 0.46              |
| 1:C:29:TYR:C     | 1:C:31:ARG:H     | 2.19                     | 0.46              |
| 1:M:169:ARG:HH22 | 1:M:221:VAL:C    | 2.19                     | 0.46              |
| 1:A:101:MET:HA   | 1:A:143:LEU:HD21 | 1.98                     | 0.46              |
| 1:L:42:THR:HA    | 2:L:299:HOH:O    | 2.15                     | 0.46              |
| 1:D:149:PRO:HA   | 1:D:152:THR:OG1  | 2.16                     | 0.46              |
| 1:K:94:GLY:HA3   | 1:K:262:VAL:HG12 | 1.97                     | 0.45              |
| 1:I:97:HIS:CG    | 1:I:262:VAL:HG21 | 2.51                     | 0.45              |
| 1:K:157:ALA:O    | 1:K:158:VAL:HB   | 2.16                     | 0.45              |
| 1:K:122:ALA:C    | 1:K:124:PHE:N    | 2.67                     | 0.45              |
| 1:J:33:LEU:O     | 1:J:34:GLU:C     | 2.54                     | 0.45              |
| 1:G:259:LEU:HD22 | 1:G:285:LEU:HD23 | 1.98                     | 0.45              |
| 1:A:99:LEU:HD12  | 1:A:100:SER:N    | 2.30                     | 0.45              |
| 1:J:22:MET:SD    | 1:J:267:ILE:CD1  | 3.04                     | 0.45              |
| 1:C:279:VAL:O    | 1:C:283:LEU:HG   | 2.15                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:190:HIS:HD2  | 1:E:248:GLU:OE1  | 1.99                     | 0.45              |
| 1:I:105:ALA:O    | 1:I:108:ALA:HB3  | 2.16                     | 0.45              |
| 1:A:135:VAL:HA   | 1:A:138:MET:SD   | 2.57                     | 0.45              |
| 1:M:245:LEU:HA   | 1:M:245:LEU:HD12 | 1.78                     | 0.45              |
| 1:L:142:VAL:O    | 1:L:145:GLY:N    | 2.49                     | 0.45              |
| 1:A:67:LEU:HD21  | 1:A:151:LEU:HG   | 1.98                     | 0.45              |
| 1:H:169:ARG:NH1  | 1:H:234:VAL:O    | 2.48                     | 0.45              |
| 1:K:35:GLN:HB2   | 1:K:283:LEU:HD21 | 1.98                     | 0.45              |
| 1:D:126:THR:HG23 | 1:D:178:LEU:CD1  | 2.46                     | 0.45              |
| 1:H:148:HIS:HD2  | 1:H:150:ARG:H    | 1.63                     | 0.45              |
| 1:C:52:SER:O     | 1:C:69:GLU:HG2   | 2.17                     | 0.45              |
| 1:C:150:ARG:HD2  | 1:C:150:ARG:HA   | 1.79                     | 0.45              |
| 1:L:189:MET:O    | 1:L:190:HIS:C    | 2.55                     | 0.45              |
| 1:A:119:ASP:HB3  | 1:A:121:HIS:O    | 2.16                     | 0.45              |
| 1:M:120:ALA:HB2  | 1:M:220:ASP:O    | 2.17                     | 0.45              |
| 1:D:135:VAL:O    | 1:D:139:PRO:HD3  | 2.17                     | 0.45              |
| 1:H:25:SER:O     | 1:H:29:TYR:CD2   | 2.61                     | 0.45              |
| 1:K:81:LEU:HD12  | 1:K:103:SER:HA   | 1.97                     | 0.45              |
| 1:J:33:LEU:O     | 1:J:36:LEU:N     | 2.48                     | 0.45              |
| 1:C:138:MET:O    | 1:C:142:VAL:HG23 | 2.17                     | 0.45              |
| 1:C:222:LEU:O    | 1:C:223:ASP:C    | 2.54                     | 0.45              |
| 1:K:128:GLU:CD   | 1:K:128:GLU:N    | 2.70                     | 0.45              |
| 1:L:270:GLU:O    | 1:L:271:ARG:HB2  | 2.17                     | 0.45              |
| 1:K:11:MET:CE    | 1:K:96:ASP:HB2   | 2.47                     | 0.45              |
| 1:L:84:LEU:HA    | 1:L:85:PRO:HD2   | 1.87                     | 0.45              |
| 1:M:179:LEU:HD13 | 1:M:186:VAL:HG21 | 1.98                     | 0.45              |
| 1:F:66:TYR:HA    | 1:F:69:GLU:OE1   | 2.17                     | 0.45              |
| 1:F:97:HIS:ND1   | 1:F:123:ASP:OD2  | 2.50                     | 0.45              |
| 1:A:97:HIS:CE1   | 1:A:117:TRP:CE2  | 3.04                     | 0.45              |
| 1:H:120:ALA:HB2  | 1:H:220:ASP:O    | 2.17                     | 0.45              |
| 1:E:94:GLY:HA3   | 1:E:99:LEU:HD21  | 1.98                     | 0.45              |
| 1:A:29:TYR:C     | 1:A:31:ARG:H     | 2.19                     | 0.45              |
| 1:E:169:ARG:HH22 | 1:E:221:VAL:C    | 2.20                     | 0.45              |
| 1:E:86:GLU:HA    | 1:E:109:ARG:HH21 | 1.81                     | 0.45              |
| 1:I:201:ALA:HB1  | 1:I:249:ILE:HG21 | 1.98                     | 0.45              |
| 1:K:70:ILE:O     | 1:K:73:ALA:N     | 2.50                     | 0.45              |
| 1:E:277:MET:HE2  | 1:E:277:MET:HB3  | 1.89                     | 0.45              |
| 1:K:8:GLY:HA3    | 1:K:48:ASP:OD1   | 2.16                     | 0.45              |
| 1:L:39:LEU:O     | 1:L:39:LEU:HG    | 2.17                     | 0.45              |
| 1:L:291:PHE:C    | 1:L:291:PHE:CD2  | 2.90                     | 0.45              |
| 1:G:169:ARG:HG3  | 1:G:234:VAL:HG11 | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:138:MET:O    | 1:I:139:PRO:C    | 2.55                     | 0.45              |
| 1:I:175:GLU:O    | 1:I:179:LEU:HB2  | 2.17                     | 0.45              |
| 1:H:231:GLY:N    | 2:H:299:HOH:O    | 2.30                     | 0.45              |
| 1:F:80:ARG:HA    | 1:F:80:ARG:HD2   | 1.60                     | 0.45              |
| 1:A:205:LEU:HD23 | 1:A:205:LEU:HA   | 1.75                     | 0.45              |
| 1:H:197:VAL:CG2  | 1:H:242:GLU:HG2  | 2.38                     | 0.45              |
| 1:M:223:ASP:OD2  | 1:M:225:THR:CG2  | 2.64                     | 0.45              |
| 1:I:125:ASN:ND2  | 1:I:129:THR:OG1  | 2.50                     | 0.45              |
| 1:L:189:MET:O    | 1:L:192:VAL:N    | 2.49                     | 0.45              |
| 1:K:149:PRO:O    | 1:K:153:GLU:HG2  | 2.17                     | 0.45              |
| 1:K:150:ARG:HA   | 1:K:153:GLU:HG2  | 1.99                     | 0.45              |
| 1:J:77:LEU:O     | 1:J:79:GLU:N     | 2.50                     | 0.45              |
| 1:I:99:LEU:HD12  | 1:I:100:SER:N    | 2.32                     | 0.45              |
| 1:J:223:ASP:OD2  | 1:J:225:THR:HB   | 2.16                     | 0.45              |
| 1:G:215:VAL:O    | 1:G:259:LEU:HA   | 2.16                     | 0.45              |
| 1:F:113:VAL:HG12 | 1:F:212:PRO:HG2  | 1.99                     | 0.45              |
| 1:L:67:LEU:C     | 1:L:67:LEU:HD23  | 2.38                     | 0.45              |
| 1:K:174:GLY:C    | 1:K:178:LEU:HD12 | 2.37                     | 0.45              |
| 1:A:79:GLU:HG2   | 1:D:111:ARG:HH21 | 1.80                     | 0.45              |
| 1:F:119:ASP:HA   | 1:F:218:ASP:HB3  | 1.99                     | 0.45              |
| 1:J:104:VAL:HB   | 1:J:143:LEU:CD2  | 2.46                     | 0.45              |
| 1:C:122:ALA:O    | 1:C:123:ASP:C    | 2.55                     | 0.45              |
| 1:F:169:ARG:HD2  | 1:F:234:VAL:CG1  | 2.47                     | 0.45              |
| 1:A:19:GLY:HA3   | 1:A:267:ILE:HD12 | 1.98                     | 0.45              |
| 1:L:82:ALA:HA    | 1:L:109:ARG:HH12 | 1.82                     | 0.44              |
| 1:L:125:ASN:HB2  | 1:L:137:GLY:O    | 2.17                     | 0.44              |
| 1:I:169:ARG:HH22 | 1:I:221:VAL:C    | 2.20                     | 0.44              |
| 1:M:34:GLU:N     | 1:M:34:GLU:CD    | 2.61                     | 0.44              |
| 1:K:169:ARG:HB3  | 1:K:189:MET:HG2  | 1.99                     | 0.44              |
| 1:I:265:ASN:HA   | 1:I:266:PRO:HD2  | 1.76                     | 0.44              |
| 1:L:159:ASP:OD1  | 1:L:160:PRO:HD2  | 2.17                     | 0.44              |
| 1:M:82:ALA:C     | 1:M:84:LEU:N     | 2.71                     | 0.44              |
| 1:I:169:ARG:HB3  | 1:I:189:MET:HG2  | 1.99                     | 0.44              |
| 1:C:97:HIS:CE1   | 1:C:117:TRP:CZ2  | 3.06                     | 0.44              |
| 1:C:19:GLY:N     | 1:C:265:ASN:ND2  | 2.61                     | 0.44              |
| 1:I:9:VAL:O      | 1:I:11:MET:N     | 2.47                     | 0.44              |
| 1:L:22:MET:SD    | 1:L:267:ILE:HD13 | 2.57                     | 0.44              |
| 1:E:20:VAL:O     | 1:E:95:GLY:HA2   | 2.17                     | 0.44              |
| 1:I:155:PHE:O    | 1:I:156:ARG:C    | 2.55                     | 0.44              |
| 1:M:126:THR:C    | 1:M:128:GLU:H    | 2.18                     | 0.44              |
| 1:L:82:ALA:HB2   | 1:L:106:GLY:O    | 2.17                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:238:LEU:HA   | 1:M:241:ARG:HH12 | 1.83                     | 0.44              |
| 1:M:24:PRO:HB2   | 2:M:294:HOH:O    | 2.17                     | 0.44              |
| 1:E:178:LEU:HA   | 1:E:178:LEU:HD23 | 1.80                     | 0.44              |
| 1:L:69:GLU:N     | 1:L:69:GLU:OE1   | 2.47                     | 0.44              |
| 1:G:140:LEU:O    | 1:G:144:SER:OG   | 2.36                     | 0.44              |
| 1:D:225:THR:HG23 | 1:D:226:LEU:N    | 2.33                     | 0.44              |
| 1:K:124:PHE:CD1  | 1:K:140:LEU:HB3  | 2.51                     | 0.44              |
| 1:E:278:LEU:O    | 1:E:281:LEU:N    | 2.49                     | 0.44              |
| 1:I:226:LEU:HD21 | 1:I:240:TYR:HB2  | 1.99                     | 0.44              |
| 1:G:229:GLY:HA3  | 1:G:269:ASP:HB2  | 1.99                     | 0.44              |
| 1:J:66:TYR:HB3   | 1:J:70:ILE:HD13  | 1.99                     | 0.44              |
| 1:A:165:LEU:HD12 | 1:A:186:VAL:HG22 | 1.99                     | 0.44              |
| 1:A:223:ASP:HA   | 1:A:224:PRO:HD3  | 1.92                     | 0.44              |
| 1:L:145:GLY:HA3  | 1:L:156:ARG:HD3  | 1.99                     | 0.44              |
| 1:J:79:GLU:O     | 1:J:81:LEU:N     | 2.51                     | 0.44              |
| 1:D:192:VAL:HA   | 1:D:200:ILE:CD1  | 2.48                     | 0.44              |
| 1:J:244:HIS:O    | 1:J:248:GLU:HG3  | 2.16                     | 0.44              |
| 1:L:289:ARG:HH11 | 1:L:289:ARG:HB2  | 1.82                     | 0.44              |
| 1:H:84:LEU:C     | 1:H:85:PRO:O     | 2.56                     | 0.44              |
| 1:F:119:ASP:OD2  | 1:F:218:ASP:OD2  | 2.35                     | 0.44              |
| 1:F:66:TYR:O     | 1:F:67:LEU:C     | 2.56                     | 0.44              |
| 1:I:129:THR:HB   | 1:I:174:GLY:HA3  | 1.99                     | 0.44              |
| 1:H:122:ALA:O    | 1:H:123:ASP:C    | 2.56                     | 0.44              |
| 1:D:214:HIS:CE1  | 1:D:260:ASP:OD2  | 2.71                     | 0.44              |
| 1:J:177:ARG:NH1  | 1:J:177:ARG:CB   | 2.80                     | 0.44              |
| 1:E:2:GLU:HB2    | 2:E:300:HOH:O    | 2.17                     | 0.44              |
| 1:I:223:ASP:OD2  | 1:I:225:THR:HG22 | 2.17                     | 0.44              |
| 1:M:10:PRO:CD    | 1:M:48:ASP:OD2   | 2.65                     | 0.44              |
| 1:K:251:ALA:O    | 1:K:254:GLY:N    | 2.40                     | 0.44              |
| 1:D:80:ARG:HD2   | 1:D:80:ARG:HA    | 1.63                     | 0.44              |
| 1:J:197:VAL:HG21 | 1:J:242:GLU:HB3  | 1.99                     | 0.44              |
| 1:H:84:LEU:O     | 1:H:85:PRO:C     | 2.55                     | 0.44              |
| 1:M:96:ASP:C     | 1:M:98:SER:H     | 2.20                     | 0.44              |
| 1:K:9:VAL:HB     | 1:K:99:LEU:CD2   | 2.48                     | 0.44              |
| 1:G:169:ARG:NH1  | 1:G:234:VAL:O    | 2.49                     | 0.44              |
| 1:C:99:LEU:HD21  | 1:C:262:VAL:HG12 | 1.98                     | 0.44              |
| 1:I:278:LEU:HD12 | 1:I:281:LEU:CD1  | 2.44                     | 0.44              |
| 1:F:164:VAL:HG11 | 1:F:204:VAL:HG22 | 2.00                     | 0.44              |
| 1:L:9:VAL:O      | 1:L:11:MET:N     | 2.50                     | 0.44              |
| 1:L:169:ARG:HG3  | 1:L:234:VAL:CG1  | 2.46                     | 0.44              |
| 1:C:32:LEU:HD11  | 1:C:36:LEU:HD11  | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:223:ASP:O    | 1:J:226:LEU:N    | 2.51                     | 0.44              |
| 1:F:37:GLU:O     | 1:F:38:ASP:C     | 2.54                     | 0.44              |
| 1:M:161:LYS:HG2  | 1:M:161:LYS:H    | 1.60                     | 0.44              |
| 1:A:277:MET:HE2  | 1:A:277:MET:HB3  | 1.85                     | 0.44              |
| 1:F:111:ARG:HH11 | 1:F:111:ARG:HG2  | 1.81                     | 0.44              |
| 1:F:97:HIS:CE1   | 1:F:117:TRP:CZ2  | 3.05                     | 0.44              |
| 1:M:226:LEU:HD21 | 1:M:240:TYR:CA   | 2.48                     | 0.44              |
| 1:M:4:VAL:HA     | 1:M:89:PHE:O     | 2.18                     | 0.44              |
| 1:I:213:LEU:HD11 | 1:I:255:ARG:HH12 | 1.82                     | 0.44              |
| 1:H:147:GLY:O    | 1:H:148:HIS:C    | 2.56                     | 0.44              |
| 1:L:144:SER:HB3  | 1:L:160:PRO:HG3  | 1.99                     | 0.44              |
| 1:G:290:ILE:N    | 1:G:290:ILE:HD12 | 2.32                     | 0.44              |
| 1:C:234:VAL:HA   | 1:C:235:PRO:HD2  | 1.80                     | 0.44              |
| 1:L:71:ARG:NH2   | 1:L:154:VAL:HG11 | 2.33                     | 0.44              |
| 1:D:22:MET:CE    | 1:J:25:SER:HB2   | 2.48                     | 0.44              |
| 1:I:46:LEU:N     | 1:I:46:LEU:HD23  | 2.33                     | 0.44              |
| 1:M:104:VAL:HG22 | 1:M:214:HIS:CE1  | 2.52                     | 0.44              |
| 1:K:112:ARG:HD3  | 1:K:211:LEU:CD2  | 2.48                     | 0.43              |
| 1:M:119:ASP:OD2  | 1:M:123:ASP:OD2  | 2.36                     | 0.43              |
| 1:M:32:LEU:HA    | 1:M:279:VAL:HG13 | 2.00                     | 0.43              |
| 1:G:29:TYR:C     | 1:G:31:ARG:H     | 2.20                     | 0.43              |
| 1:J:126:THR:O    | 1:J:127:PRO:C    | 2.56                     | 0.43              |
| 1:C:264:VAL:CG2  | 1:C:278:LEU:HD22 | 2.48                     | 0.43              |
| 1:C:188:THR:O    | 1:C:192:VAL:HG23 | 2.18                     | 0.43              |
| 1:M:224:PRO:CG   | 1:M:233:PRO:HB2  | 2.48                     | 0.43              |
| 1:G:97:HIS:ND1   | 1:G:119:ASP:OD2  | 2.51                     | 0.43              |
| 1:J:148:HIS:HA   | 1:J:149:PRO:HD3  | 1.82                     | 0.43              |
| 1:H:13:LEU:CB    | 1:H:70:ILE:HD11  | 2.47                     | 0.43              |
| 1:A:199:ARG:HA   | 1:A:202:GLU:HG3  | 1.99                     | 0.43              |
| 1:K:124:PHE:O    | 1:K:175:GLU:HG2  | 2.18                     | 0.43              |
| 1:D:169:ARG:HB3  | 1:D:189:MET:HG2  | 1.99                     | 0.43              |
| 1:D:169:ARG:NH2  | 1:D:237:GLY:CA   | 2.80                     | 0.43              |
| 1:I:153:GLU:HG3  | 1:I:154:VAL:HG13 | 2.01                     | 0.43              |
| 1:G:97:HIS:CE1   | 1:G:119:ASP:OD2  | 2.71                     | 0.43              |
| 1:J:100:SER:O    | 1:J:101:MET:C    | 2.57                     | 0.43              |
| 1:L:172:ASP:O    | 1:L:175:GLU:HB2  | 2.18                     | 0.43              |
| 1:D:104:VAL:CG2  | 1:D:214:HIS:CE1  | 2.99                     | 0.43              |
| 1:G:32:LEU:HD12  | 1:G:279:VAL:HG13 | 2.00                     | 0.43              |
| 1:H:279:VAL:O    | 1:H:283:LEU:HG   | 2.18                     | 0.43              |
| 1:H:227:ALA:HB1  | 1:H:274:THR:HG23 | 2.00                     | 0.43              |
| 1:L:113:VAL:HB   | 1:L:212:PRO:O    | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:109:ARG:NH1  | 1:F:109:ARG:HG2  | 2.32                     | 0.43              |
| 1:M:80:ARG:CG    | 1:M:80:ARG:NH1   | 2.69                     | 0.43              |
| 1:L:247:MET:SD   | 1:L:285:LEU:HD22 | 2.58                     | 0.43              |
| 1:G:129:THR:O    | 1:G:130:SER:CB   | 2.66                     | 0.43              |
| 1:J:165:LEU:HD12 | 1:J:186:VAL:HG22 | 2.00                     | 0.43              |
| 1:J:77:LEU:C     | 1:J:79:GLU:N     | 2.71                     | 0.43              |
| 1:M:3:ARG:HH12   | 1:M:85:PRO:HB2   | 1.84                     | 0.43              |
| 1:A:229:GLY:HA3  | 1:A:269:ASP:HB2  | 2.00                     | 0.43              |
| 1:G:118:VAL:HB   | 1:G:217:LEU:HD12 | 1.99                     | 0.43              |
| 1:F:13:LEU:N     | 1:F:96:ASP:OD2   | 2.43                     | 0.43              |
| 1:K:69:GLU:O     | 1:K:72:ALA:HB3   | 2.18                     | 0.43              |
| 1:I:78:LYS:HE3   | 1:I:105:ALA:HB1  | 2.00                     | 0.43              |
| 1:E:187:TYR:CD1  | 1:E:200:ILE:HG12 | 2.54                     | 0.43              |
| 1:D:264:VAL:CG2  | 1:D:278:LEU:HD22 | 2.48                     | 0.43              |
| 1:A:123:ASP:HB3  | 1:A:139:PRO:HG2  | 2.01                     | 0.43              |
| 1:L:262:VAL:O    | 1:L:263:GLU:HB2  | 2.18                     | 0.43              |
| 1:F:169:ARG:CZ   | 1:F:237:GLY:HA2  | 2.48                     | 0.43              |
| 1:D:43:VAL:CG1   | 1:D:44:GLU:H     | 2.32                     | 0.43              |
| 1:E:290:ILE:N    | 1:E:290:ILE:HD12 | 2.33                     | 0.43              |
| 1:K:124:PHE:HD1  | 1:K:140:LEU:CB   | 2.30                     | 0.43              |
| 1:C:98:SER:O     | 1:C:101:MET:HG3  | 2.18                     | 0.43              |
| 1:E:169:ARG:NH2  | 1:E:221:VAL:O    | 2.51                     | 0.43              |
| 1:J:225:THR:HG22 | 1:J:226:LEU:N    | 2.33                     | 0.43              |
| 1:K:222:LEU:O    | 1:K:223:ASP:C    | 2.56                     | 0.43              |
| 1:J:145:GLY:HA2  | 1:J:156:ARG:HG3  | 2.00                     | 0.43              |
| 1:F:122:ALA:O    | 1:F:124:PHE:N    | 2.52                     | 0.43              |
| 1:J:70:ILE:N     | 1:J:70:ILE:HD12  | 2.34                     | 0.43              |
| 1:J:214:HIS:CD2  | 1:J:258:SER:OG   | 2.72                     | 0.43              |
| 1:K:96:ASP:C     | 1:K:98:SER:H     | 2.21                     | 0.43              |
| 1:L:173:PRO:O    | 1:L:176:LYS:HB2  | 2.19                     | 0.43              |
| 1:C:269:ASP:OD1  | 1:C:270:GLU:N    | 2.46                     | 0.43              |
| 1:L:190:HIS:CE1  | 1:L:194:ARG:HE   | 2.19                     | 0.43              |
| 1:L:186:VAL:O    | 1:L:186:VAL:CG1  | 2.67                     | 0.43              |
| 1:F:169:ARG:HD2  | 1:F:234:VAL:HG12 | 2.01                     | 0.43              |
| 1:C:246:LEU:O    | 1:C:250:LEU:HG   | 2.19                     | 0.43              |
| 1:K:253:SER:C    | 1:K:255:ARG:N    | 2.72                     | 0.43              |
| 1:K:12:ASP:O     | 1:K:13:LEU:HD23  | 2.19                     | 0.43              |
| 1:I:278:LEU:HA   | 1:I:281:LEU:HD12 | 2.00                     | 0.43              |
| 1:M:172:ASP:O    | 1:M:176:LYS:HG3  | 2.19                     | 0.43              |
| 1:E:226:LEU:HD11 | 1:E:240:TYR:HB2  | 2.01                     | 0.43              |
| 1:A:256:VAL:HG21 | 1:A:285:LEU:CD1  | 2.48                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:243:ALA:HB1  | 1:K:281:LEU:CD1  | 2.47                     | 0.43              |
| 1:E:11:MET:CE    | 1:E:98:SER:HB2   | 2.49                     | 0.43              |
| 1:G:164:VAL:HG11 | 1:G:204:VAL:HG22 | 2.00                     | 0.43              |
| 1:E:119:ASP:OD1  | 1:E:220:ASP:OD2  | 2.36                     | 0.43              |
| 1:C:129:THR:O    | 1:C:130:SER:HB3  | 2.18                     | 0.43              |
| 1:J:251:ALA:HB2  | 1:J:285:LEU:HA   | 2.01                     | 0.43              |
| 1:A:201:ALA:HB1  | 1:A:249:ILE:HG21 | 2.01                     | 0.43              |
| 1:A:177:ARG:HH11 | 1:A:177:ARG:HG2  | 1.83                     | 0.43              |
| 1:L:6:VAL:O      | 1:L:6:VAL:HG12   | 2.18                     | 0.43              |
| 1:J:24:PRO:O     | 1:J:28:ARG:HG3   | 2.19                     | 0.43              |
| 1:M:80:ARG:HG2   | 1:M:80:ARG:NH1   | 2.17                     | 0.42              |
| 1:L:247:MET:HA   | 1:L:285:LEU:HD13 | 2.00                     | 0.42              |
| 1:M:124:PHE:CA   | 1:M:141:ALA:HB2  | 2.49                     | 0.42              |
| 1:M:146:LEU:CD1  | 1:M:178:LEU:HD22 | 2.43                     | 0.42              |
| 1:A:197:VAL:HG21 | 1:A:242:GLU:HB3  | 2.00                     | 0.42              |
| 1:C:199:ARG:HA   | 1:C:202:GLU:HG3  | 2.01                     | 0.42              |
| 1:M:201:ALA:CB   | 1:M:249:ILE:HG21 | 2.50                     | 0.42              |
| 1:E:3:ARG:HB3    | 1:E:88:VAL:HG22  | 2.01                     | 0.42              |
| 1:E:185:ARG:HG2  | 1:E:185:ARG:NH1  | 2.34                     | 0.42              |
| 1:J:5:ALA:HA     | 1:J:44:GLU:O     | 2.19                     | 0.42              |
| 1:G:218:ASP:O    | 1:G:221:VAL:HG12 | 2.18                     | 0.42              |
| 1:M:84:LEU:O     | 1:M:109:ARG:NH2  | 2.52                     | 0.42              |
| 1:L:215:VAL:O    | 1:L:259:LEU:HA   | 2.19                     | 0.42              |
| 1:D:95:GLY:O     | 1:D:96:ASP:C     | 2.58                     | 0.42              |
| 1:M:3:ARG:NH1    | 1:M:85:PRO:HB2   | 2.35                     | 0.42              |
| 1:L:291:PHE:OXT  | 1:L:291:PHE:HD2  | 2.02                     | 0.42              |
| 1:I:207:HIS:O    | 1:I:207:HIS:CG   | 2.72                     | 0.42              |
| 1:K:165:LEU:HB2  | 1:K:186:VAL:HG22 | 2.00                     | 0.42              |
| 1:J:204:VAL:C    | 1:J:206:LYS:H    | 2.22                     | 0.42              |
| 1:L:124:PHE:CD2  | 1:L:179:LEU:HG   | 2.54                     | 0.42              |
| 1:A:25:SER:HB2   | 1:H:22:MET:CE    | 2.49                     | 0.42              |
| 1:H:148:HIS:CD2  | 1:H:150:ARG:HB2  | 2.55                     | 0.42              |
| 1:L:275:ALA:O    | 1:L:276:GLU:C    | 2.58                     | 0.42              |
| 1:M:25:SER:O     | 1:M:28:ARG:HB2   | 2.19                     | 0.42              |
| 1:I:245:LEU:O    | 1:I:245:LEU:HG   | 2.15                     | 0.42              |
| 1:M:148:HIS:CD2  | 1:M:150:ARG:H    | 2.36                     | 0.42              |
| 1:H:251:ALA:HB2  | 1:H:285:LEU:HA   | 2.01                     | 0.42              |
| 1:L:177:ARG:C    | 1:L:179:LEU:H    | 2.21                     | 0.42              |
| 1:J:169:ARG:HG3  | 1:J:234:VAL:CG1  | 2.49                     | 0.42              |
| 1:J:22:MET:HB2   | 1:J:266:PRO:HG2  | 2.01                     | 0.42              |
| 1:J:89:PHE:HA    | 1:J:90:PRO:HD3   | 1.89                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:168:VAL:CG1  | 1:I:171:LEU:HD21 | 2.49                     | 0.42              |
| 1:D:25:SER:O     | 1:D:29:TYR:HD2   | 2.03                     | 0.42              |
| 1:M:165:LEU:CB   | 1:M:186:VAL:HG22 | 2.49                     | 0.42              |
| 1:L:90:PRO:HG2   | 1:L:258:SER:HB3  | 2.02                     | 0.42              |
| 1:M:240:TYR:HD1  | 1:M:277:MET:SD   | 2.42                     | 0.42              |
| 1:L:126:THR:C    | 1:L:128:GLU:N    | 2.73                     | 0.42              |
| 1:I:20:VAL:CG1   | 1:I:265:ASN:HB2  | 2.48                     | 0.42              |
| 1:E:108:ALA:O    | 1:E:109:ARG:HB2  | 2.19                     | 0.42              |
| 1:H:164:VAL:HG11 | 1:H:204:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:278:LEU:O    | 1:A:279:VAL:C    | 2.58                     | 0.42              |
| 1:G:70:ILE:O     | 1:G:71:ARG:C     | 2.56                     | 0.42              |
| 1:H:111:ARG:HE   | 1:H:112:ARG:N    | 2.17                     | 0.42              |
| 1:M:11:MET:O     | 1:M:96:ASP:N     | 2.50                     | 0.42              |
| 1:J:145:GLY:C    | 1:J:146:LEU:HD23 | 2.39                     | 0.42              |
| 1:C:155:PHE:O    | 1:C:156:ARG:C    | 2.55                     | 0.42              |
| 1:H:101:MET:HG3  | 1:H:139:PRO:HB3  | 2.02                     | 0.42              |
| 1:K:221:VAL:HG22 | 1:K:221:VAL:O    | 2.20                     | 0.42              |
| 1:H:149:PRO:C    | 1:H:151:LEU:N    | 2.73                     | 0.42              |
| 1:F:74:ALA:O     | 1:F:77:LEU:HB3   | 2.19                     | 0.42              |
| 1:G:39:LEU:HD12  | 1:G:39:LEU:HA    | 1.75                     | 0.42              |
| 1:E:22:MET:SD    | 1:E:267:ILE:CD1  | 3.08                     | 0.42              |
| 1:M:220:ASP:OD1  | 1:M:220:ASP:C    | 2.58                     | 0.42              |
| 1:L:120:ALA:HB2  | 1:L:220:ASP:O    | 2.19                     | 0.42              |
| 1:L:118:VAL:HG13 | 1:L:166:VAL:HB   | 2.01                     | 0.42              |
| 1:L:126:THR:CG2  | 1:L:178:LEU:HD13 | 2.49                     | 0.42              |
| 1:D:64:LEU:O     | 1:D:67:LEU:HB2   | 2.20                     | 0.42              |
| 1:L:36:LEU:HD22  | 1:L:286:LEU:HD23 | 2.02                     | 0.42              |
| 1:F:35:GLN:HB3   | 1:F:283:LEU:HD11 | 2.02                     | 0.42              |
| 1:G:5:ALA:O      | 1:G:90:PRO:HA    | 2.19                     | 0.42              |
| 1:J:179:LEU:HD23 | 1:J:184:VAL:HG21 | 2.02                     | 0.42              |
| 1:A:111:ARG:NE   | 1:A:111:ARG:HA   | 2.35                     | 0.42              |
| 1:M:211:LEU:HD23 | 1:M:211:LEU:N    | 2.35                     | 0.42              |
| 1:F:95:GLY:O     | 1:F:96:ASP:O     | 2.38                     | 0.42              |
| 1:M:218:ASP:CG   | 1:M:263:GLU:HG3  | 2.40                     | 0.42              |
| 1:J:249:ILE:HD13 | 1:J:249:ILE:HA   | 1.75                     | 0.42              |
| 1:F:169:ARG:HH11 | 1:F:234:VAL:HB   | 1.85                     | 0.42              |
| 1:A:9:VAL:O      | 1:A:11:MET:N     | 2.52                     | 0.42              |
| 1:A:192:VAL:HA   | 1:A:200:ILE:CD1  | 2.49                     | 0.42              |
| 1:K:219:ALA:C    | 1:K:221:VAL:H    | 2.22                     | 0.42              |
| 1:A:269:ASP:CG   | 1:A:270:GLU:H    | 2.23                     | 0.42              |
| 1:H:32:LEU:HA    | 1:H:279:VAL:CG1  | 2.49                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:202:GLU:HG2  | 1:E:202:GLU:H    | 1.66                     | 0.42              |
| 1:H:104:VAL:HG22 | 1:H:214:HIS:CE1  | 2.55                     | 0.42              |
| 1:H:82:ALA:CA    | 1:H:109:ARG:HH12 | 2.24                     | 0.42              |
| 1:L:37:GLU:HG2   | 1:L:43:VAL:HG23  | 2.01                     | 0.42              |
| 1:I:278:LEU:HA   | 1:I:278:LEU:HD12 | 1.75                     | 0.42              |
| 1:A:202:GLU:H    | 1:A:202:GLU:HG2  | 1.63                     | 0.42              |
| 1:L:163:VAL:HB   | 1:L:184:VAL:HG13 | 2.01                     | 0.42              |
| 1:L:177:ARG:O    | 1:L:181:GLU:HB2  | 2.20                     | 0.42              |
| 1:M:256:VAL:HG11 | 1:M:285:LEU:HD21 | 2.01                     | 0.42              |
| 1:C:125:ASN:ND2  | 1:C:129:THR:OG1  | 2.52                     | 0.42              |
| 1:H:69:GLU:O     | 1:H:72:ALA:HB3   | 2.19                     | 0.42              |
| 1:F:126:THR:HG23 | 1:F:178:LEU:HD13 | 2.00                     | 0.42              |
| 1:I:34:GLU:H     | 1:I:34:GLU:CD    | 2.22                     | 0.42              |
| 1:J:206:LYS:C    | 1:J:208:LEU:H    | 2.23                     | 0.42              |
| 1:M:99:LEU:HD12  | 1:M:100:SER:N    | 2.34                     | 0.42              |
| 1:C:129:THR:HB   | 1:C:174:GLY:HA3  | 2.02                     | 0.42              |
| 1:E:177:ARG:CB   | 1:E:177:ARG:NH1  | 2.81                     | 0.42              |
| 1:J:89:PHE:HE1   | 1:J:256:VAL:O    | 2.03                     | 0.42              |
| 1:K:275:ALA:O    | 1:K:276:GLU:C    | 2.58                     | 0.42              |
| 1:H:163:VAL:CG1  | 1:H:164:VAL:N    | 2.83                     | 0.42              |
| 1:F:36:LEU:O     | 1:F:39:LEU:N     | 2.53                     | 0.42              |
| 1:G:201:ALA:CB   | 1:G:249:ILE:HG21 | 2.49                     | 0.41              |
| 1:M:140:LEU:HD23 | 1:M:165:LEU:HD11 | 2.01                     | 0.41              |
| 1:C:271:ARG:CZ   | 1:K:268:LEU:O    | 2.68                     | 0.41              |
| 1:K:94:GLY:N     | 1:K:261:LEU:O    | 2.44                     | 0.41              |
| 1:I:119:ASP:HA   | 1:I:218:ASP:HB3  | 2.02                     | 0.41              |
| 1:J:115:VAL:CG2  | 1:J:158:VAL:HG21 | 2.50                     | 0.41              |
| 1:K:226:LEU:HD21 | 1:K:240:TYR:CA   | 2.49                     | 0.41              |
| 1:H:234:VAL:HA   | 1:H:235:PRO:HD2  | 1.81                     | 0.41              |
| 1:F:113:VAL:HG11 | 1:F:257:GLN:NE2  | 2.35                     | 0.41              |
| 1:M:214:HIS:CD2  | 1:M:258:SER:HB2  | 2.55                     | 0.41              |
| 1:G:71:ARG:NH2   | 1:G:153:GLU:OE2  | 2.51                     | 0.41              |
| 1:D:261:LEU:HD11 | 1:D:282:ALA:HB2  | 2.01                     | 0.41              |
| 1:H:116:VAL:HB   | 1:H:215:VAL:HG22 | 2.01                     | 0.41              |
| 1:K:119:ASP:HA   | 1:K:218:ASP:HB3  | 2.01                     | 0.41              |
| 1:E:121:HIS:HE1  | 1:E:232:THR:HB   | 1.85                     | 0.41              |
| 1:J:6:VAL:CG1    | 1:J:93:LEU:HD21  | 2.47                     | 0.41              |
| 1:M:91:ILE:HG23  | 1:M:259:LEU:HD23 | 2.01                     | 0.41              |
| 1:C:111:ARG:CD   | 1:C:112:ARG:N    | 2.82                     | 0.41              |
| 1:D:39:LEU:HD12  | 1:D:39:LEU:HA    | 1.84                     | 0.41              |
| 1:G:227:ALA:N    | 1:G:228:PRO:HD3  | 2.34                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:138:MET:C    | 2:L:301:HOH:O    | 2.58                     | 0.41              |
| 1:M:119:ASP:OD2  | 1:M:218:ASP:OD2  | 2.38                     | 0.41              |
| 1:M:99:LEU:C     | 1:M:99:LEU:HD12  | 2.41                     | 0.41              |
| 1:H:12:ASP:O     | 1:H:13:LEU:HD23  | 2.21                     | 0.41              |
| 1:L:20:VAL:C     | 1:L:22:MET:H     | 2.23                     | 0.41              |
| 1:C:252:GLU:OE2  | 1:I:194:ARG:NH2  | 2.53                     | 0.41              |
| 1:K:277:MET:CE   | 1:K:277:MET:CA   | 2.98                     | 0.41              |
| 1:K:22:MET:SD    | 1:K:267:ILE:CD1  | 3.09                     | 0.41              |
| 1:G:168:VAL:HG12 | 1:G:188:THR:HG22 | 2.02                     | 0.41              |
| 1:D:148:HIS:CD2  | 1:D:150:ARG:H    | 2.38                     | 0.41              |
| 1:J:160:PRO:C    | 1:J:162:ASP:H    | 2.24                     | 0.41              |
| 1:L:99:LEU:HD12  | 1:L:99:LEU:C     | 2.40                     | 0.41              |
| 1:I:124:PHE:O    | 1:I:124:PHE:CD2  | 2.73                     | 0.41              |
| 1:M:39:LEU:HA    | 1:M:39:LEU:HD12  | 1.75                     | 0.41              |
| 1:L:89:PHE:CZ    | 1:L:256:VAL:HG12 | 2.52                     | 0.41              |
| 1:J:139:PRO:O    | 1:J:143:LEU:HD12 | 2.20                     | 0.41              |
| 1:J:119:ASP:HB3  | 1:J:121:HIS:O    | 2.19                     | 0.41              |
| 1:F:265:ASN:HA   | 1:F:266:PRO:HD2  | 1.93                     | 0.41              |
| 1:I:265:ASN:ND2  | 1:I:268:LEU:HG   | 2.36                     | 0.41              |
| 1:K:35:GLN:OE1   | 1:K:283:LEU:HD11 | 2.19                     | 0.41              |
| 1:J:247:MET:SD   | 1:J:285:LEU:HD13 | 2.61                     | 0.41              |
| 1:H:3:ARG:HB2    | 1:H:3:ARG:HE     | 1.59                     | 0.41              |
| 1:C:84:LEU:O     | 1:C:85:PRO:C     | 2.58                     | 0.41              |
| 1:G:139:PRO:O    | 1:G:143:LEU:HG   | 2.20                     | 0.41              |
| 1:F:9:VAL:O      | 1:F:11:MET:N     | 2.53                     | 0.41              |
| 1:A:97:HIS:CD2   | 1:A:262:VAL:HG21 | 2.56                     | 0.41              |
| 1:K:193:ASP:HB2  | 1:M:245:LEU:HD13 | 2.01                     | 0.41              |
| 1:E:153:GLU:HG3  | 1:E:154:VAL:N    | 2.35                     | 0.41              |
| 1:K:148:HIS:HA   | 1:K:149:PRO:HD3  | 1.85                     | 0.41              |
| 1:E:34:GLU:OE1   | 1:E:34:GLU:N     | 2.34                     | 0.41              |
| 1:L:93:LEU:HD22  | 1:L:261:LEU:HD12 | 2.03                     | 0.41              |
| 1:D:234:VAL:HA   | 1:D:235:PRO:HD3  | 1.91                     | 0.41              |
| 1:G:32:LEU:CD1   | 1:G:279:VAL:HG13 | 2.50                     | 0.41              |
| 1:L:277:MET:CE   | 1:L:277:MET:HA   | 2.51                     | 0.41              |
| 1:I:288:LYS:O    | 1:I:289:ARG:HG3  | 2.21                     | 0.41              |
| 1:F:168:VAL:HG11 | 1:F:171:LEU:HD21 | 2.02                     | 0.41              |
| 1:H:199:ARG:O    | 1:H:200:ILE:C    | 2.57                     | 0.41              |
| 1:M:13:LEU:HD12  | 1:M:70:ILE:CG1   | 2.42                     | 0.41              |
| 1:C:148:HIS:CD2  | 1:C:150:ARG:HB2  | 2.56                     | 0.41              |
| 1:C:67:LEU:HD21  | 1:C:150:ARG:HB2  | 2.02                     | 0.41              |
| 1:E:37:GLU:HG2   | 1:E:43:VAL:CG2   | 2.42                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:22:MET:HE1   | 1:H:25:SER:HB2   | 2.03                     | 0.41              |
| 1:K:190:HIS:O    | 1:K:194:ARG:HB2  | 2.21                     | 0.41              |
| 1:M:243:ALA:HB1  | 1:M:281:LEU:CD1  | 2.50                     | 0.41              |
| 1:G:11:MET:O     | 1:G:96:ASP:OD2   | 2.39                     | 0.41              |
| 1:C:248:GLU:OE1  | 1:I:190:HIS:CD2  | 2.68                     | 0.41              |
| 1:H:146:LEU:HD23 | 1:H:146:LEU:N    | 2.36                     | 0.41              |
| 1:G:94:GLY:HA3   | 1:G:99:LEU:CD2   | 2.50                     | 0.41              |
| 1:G:22:MET:CB    | 1:G:266:PRO:HG2  | 2.51                     | 0.41              |
| 1:D:171:LEU:HB2  | 1:D:176:LYS:HE2  | 2.03                     | 0.41              |
| 1:M:150:ARG:CD   | 1:M:150:ARG:O    | 2.67                     | 0.41              |
| 1:A:117:TRP:HB3  | 1:A:165:LEU:HD23 | 2.03                     | 0.41              |
| 1:M:286:LEU:CD1  | 1:M:286:LEU:N    | 2.83                     | 0.41              |
| 1:M:172:ASP:HB3  | 1:M:173:PRO:HD2  | 2.03                     | 0.41              |
| 1:I:225:THR:O    | 1:I:273:ARG:NH2  | 2.54                     | 0.41              |
| 1:L:64:LEU:HD13  | 1:L:65:ALA:H     | 1.84                     | 0.41              |
| 1:G:265:ASN:OD1  | 1:G:267:ILE:HB   | 2.20                     | 0.41              |
| 1:F:46:LEU:HD13  | 1:F:80:ARG:NH2   | 2.35                     | 0.41              |
| 1:I:159:ASP:C    | 1:I:159:ASP:OD1  | 2.59                     | 0.41              |
| 1:M:150:ARG:O    | 1:M:153:GLU:OE2  | 2.38                     | 0.41              |
| 1:M:243:ALA:O    | 1:M:247:MET:HG2  | 2.21                     | 0.41              |
| 1:A:67:LEU:HD11  | 1:A:148:HIS:CG   | 2.55                     | 0.41              |
| 1:E:109:ARG:C    | 1:E:111:ARG:H    | 2.24                     | 0.41              |
| 1:C:259:LEU:HD13 | 1:C:285:LEU:HD22 | 2.03                     | 0.41              |
| 1:M:217:LEU:HA   | 1:M:217:LEU:HD12 | 1.85                     | 0.41              |
| 1:J:208:LEU:HD23 | 1:J:208:LEU:HA   | 1.91                     | 0.41              |
| 1:J:145:GLY:CA   | 1:J:156:ARG:HD2  | 2.51                     | 0.41              |
| 1:F:67:LEU:O     | 1:F:71:ARG:HB2   | 2.21                     | 0.41              |
| 1:J:100:SER:C    | 1:J:103:SER:HG   | 2.23                     | 0.41              |
| 1:J:99:LEU:C     | 1:J:99:LEU:CD1   | 2.82                     | 0.41              |
| 1:E:37:GLU:HA    | 1:E:41:TYR:O     | 2.20                     | 0.41              |
| 1:M:218:ASP:OD1  | 1:M:263:GLU:HB2  | 2.21                     | 0.41              |
| 1:M:99:LEU:HD21  | 1:M:262:VAL:HG12 | 2.03                     | 0.41              |
| 1:J:168:VAL:CG1  | 1:J:171:LEU:HD21 | 2.45                     | 0.41              |
| 1:J:140:LEU:HD23 | 1:J:165:LEU:HD21 | 2.03                     | 0.41              |
| 1:I:163:VAL:HG12 | 1:I:184:VAL:HG13 | 2.03                     | 0.41              |
| 1:H:12:ASP:HB3   | 1:H:21:ASP:HB3   | 2.03                     | 0.41              |
| 1:D:99:LEU:HD21  | 1:D:262:VAL:CG1  | 2.47                     | 0.41              |
| 1:L:97:HIS:ND1   | 1:L:119:ASP:OD2  | 2.53                     | 0.41              |
| 1:G:11:MET:O     | 1:G:96:ASP:CG    | 2.59                     | 0.41              |
| 1:K:176:LYS:HD3  | 1:M:291:PHE:HD2  | 1.85                     | 0.41              |
| 1:C:96:ASP:HB3   | 1:C:136:HIS:HB3  | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:168:VAL:HG11 | 1:I:171:LEU:HD21 | 2.03                     | 0.41              |
| 1:K:75:LEU:HG    | 1:K:79:GLU:HG3   | 2.03                     | 0.41              |
| 1:K:4:VAL:HG22   | 1:K:89:PHE:HB3   | 2.03                     | 0.41              |
| 1:K:185:ARG:NH1  | 1:K:207:HIS:ND1  | 2.69                     | 0.41              |
| 1:I:153:GLU:CG   | 1:I:154:VAL:HG13 | 2.51                     | 0.41              |
| 1:L:10:PRO:O     | 1:L:51:VAL:HG21  | 2.20                     | 0.41              |
| 1:H:159:ASP:O    | 1:H:162:ASP:N    | 2.47                     | 0.41              |
| 1:G:72:ALA:O     | 1:G:76:VAL:HG23  | 2.20                     | 0.41              |
| 1:F:277:MET:HB3  | 1:F:277:MET:HE2  | 2.00                     | 0.41              |
| 1:M:128:GLU:C    | 1:M:130:SER:N    | 2.74                     | 0.41              |
| 1:J:138:MET:H    | 1:J:139:PRO:HD2  | 1.76                     | 0.41              |
| 1:H:135:VAL:O    | 1:H:138:MET:N    | 2.46                     | 0.41              |
| 1:M:194:ARG:CG   | 1:M:194:ARG:HH11 | 2.33                     | 0.41              |
| 1:K:169:ARG:CZ   | 1:K:237:GLY:HA3  | 2.51                     | 0.41              |
| 1:J:79:GLU:C     | 1:J:81:LEU:N     | 2.74                     | 0.41              |
| 1:J:278:LEU:HD12 | 1:J:278:LEU:HA   | 1.84                     | 0.41              |
| 1:F:111:ARG:NH2  | 1:G:249:ILE:O    | 2.54                     | 0.40              |
| 1:F:211:LEU:H    | 1:F:255:ARG:NH1  | 2.19                     | 0.40              |
| 1:C:84:LEU:HG    | 1:C:84:LEU:H     | 1.67                     | 0.40              |
| 1:M:82:ALA:O     | 1:M:84:LEU:N     | 2.48                     | 0.40              |
| 1:F:67:LEU:HD21  | 1:F:150:ARG:HB2  | 2.03                     | 0.40              |
| 1:I:232:THR:O    | 1:I:233:PRO:C    | 2.60                     | 0.40              |
| 1:L:202:GLU:OE1  | 1:L:202:GLU:HA   | 2.21                     | 0.40              |
| 1:L:205:LEU:O    | 1:L:255:ARG:NH2  | 2.54                     | 0.40              |
| 1:F:145:GLY:CA   | 1:F:156:ARG:HD3  | 2.47                     | 0.40              |
| 1:L:81:LEU:HD12  | 1:L:103:SER:HA   | 2.02                     | 0.40              |
| 1:D:89:PHE:CZ    | 1:D:286:LEU:HD11 | 2.56                     | 0.40              |
| 1:E:223:ASP:HA   | 1:E:224:PRO:HD3  | 1.96                     | 0.40              |
| 1:E:125:ASN:HB2  | 1:E:137:GLY:O    | 2.21                     | 0.40              |
| 1:K:39:LEU:HA    | 1:K:39:LEU:HD12  | 1.60                     | 0.40              |
| 1:J:153:GLU:HG3  | 1:J:154:VAL:HG13 | 2.02                     | 0.40              |
| 1:J:156:ARG:O    | 1:J:157:ALA:HB2  | 2.21                     | 0.40              |
| 1:F:11:MET:HE1   | 1:F:70:ILE:HG23  | 2.04                     | 0.40              |
| 1:L:285:LEU:HA   | 1:L:285:LEU:HD12 | 1.84                     | 0.40              |
| 1:H:12:ASP:CB    | 1:H:21:ASP:HB3   | 2.51                     | 0.40              |
| 1:A:29:TYR:CE1   | 1:H:19:GLY:HA2   | 2.57                     | 0.40              |
| 1:I:71:ARG:CZ    | 1:I:150:ARG:NH1  | 2.84                     | 0.40              |
| 1:A:19:GLY:N     | 1:A:265:ASN:HD21 | 2.20                     | 0.40              |
| 1:I:206:LYS:C    | 1:I:208:LEU:H    | 2.25                     | 0.40              |
| 1:A:288:LYS:O    | 1:A:289:ARG:HG3  | 2.20                     | 0.40              |
| 1:G:135:VAL:C    | 1:G:137:GLY:H    | 2.24                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:145:GLY:HA2  | 1:J:156:ARG:CG   | 2.52                     | 0.40              |
| 1:K:67:LEU:HA    | 1:K:70:ILE:HD12  | 2.03                     | 0.40              |
| 1:H:138:MET:H    | 1:H:139:PRO:HD2  | 1.86                     | 0.40              |
| 1:A:86:GLU:HB2   | 1:D:86:GLU:HG3   | 2.02                     | 0.40              |
| 1:E:112:ARG:CZ   | 1:E:211:LEU:HD21 | 2.51                     | 0.40              |
| 1:M:214:HIS:CD2  | 1:M:258:SER:OG   | 2.74                     | 0.40              |
| 1:A:227:ALA:O    | 1:A:230:VAL:HG13 | 2.21                     | 0.40              |
| 1:D:112:ARG:HH11 | 1:D:211:LEU:HD21 | 1.84                     | 0.40              |
| 1:K:97:HIS:CE1   | 1:K:117:TRP:CZ2  | 3.10                     | 0.40              |
| 1:D:204:VAL:HG12 | 1:D:204:VAL:O    | 2.20                     | 0.40              |
| 1:G:30:ALA:HB3   | 1:G:279:VAL:HG21 | 2.04                     | 0.40              |
| 1:L:79:GLU:O     | 1:L:81:LEU:N     | 2.54                     | 0.40              |
| 1:H:37:GLU:HA    | 1:H:41:TYR:O     | 2.21                     | 0.40              |
| 1:A:111:ARG:NH2  | 1:D:79:GLU:O     | 2.28                     | 0.40              |
| 1:F:129:THR:O    | 1:F:130:SER:CB   | 2.69                     | 0.40              |
| 1:L:90:PRO:C     | 1:L:91:ILE:HD13  | 2.42                     | 0.40              |
| 1:D:98:SER:HA    | 1:D:139:PRO:HG3  | 2.04                     | 0.40              |
| 1:F:225:THR:HG22 | 1:F:226:LEU:N    | 2.35                     | 0.40              |
| 1:M:283:LEU:O    | 1:M:288:LYS:CB   | 2.69                     | 0.40              |
| 1:L:104:VAL:HG21 | 1:L:143:LEU:CD1  | 2.52                     | 0.40              |
| 1:M:209:GLN:HA   | 1:M:255:ARG:NH2  | 2.37                     | 0.40              |
| 1:L:79:GLU:O     | 1:L:80:ARG:C     | 2.60                     | 0.40              |
| 1:J:225:THR:CG2  | 1:J:226:LEU:N    | 2.82                     | 0.40              |
| 1:J:202:GLU:HG2  | 1:J:202:GLU:H    | 1.67                     | 0.40              |
| 1:M:198:ALA:C    | 1:M:200:ILE:H    | 2.25                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 265/291 (91%) | 246 (93%) | 17 (6%) | 2 (1%)   | 24          | 58 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | C     | 265/291 (91%)   | 245 (92%)  | 18 (7%)   | 2 (1%)   | 24          | 58 |
| 1   | D     | 265/291 (91%)   | 248 (94%)  | 14 (5%)   | 3 (1%)   | 17          | 50 |
| 1   | E     | 265/291 (91%)   | 236 (89%)  | 25 (9%)   | 4 (2%)   | 13          | 41 |
| 1   | F     | 265/291 (91%)   | 242 (91%)  | 19 (7%)   | 4 (2%)   | 13          | 41 |
| 1   | G     | 265/291 (91%)   | 231 (87%)  | 32 (12%)  | 2 (1%)   | 24          | 58 |
| 1   | H     | 265/291 (91%)   | 240 (91%)  | 21 (8%)   | 4 (2%)   | 13          | 41 |
| 1   | I     | 265/291 (91%)   | 225 (85%)  | 34 (13%)  | 6 (2%)   | 8           | 29 |
| 1   | J     | 265/291 (91%)   | 217 (82%)  | 37 (14%)  | 11 (4%)  | 3           | 12 |
| 1   | K     | 265/291 (91%)   | 206 (78%)  | 50 (19%)  | 9 (3%)   | 5           | 18 |
| 1   | L     | 265/291 (91%)   | 220 (83%)  | 34 (13%)  | 11 (4%)  | 3           | 12 |
| 1   | M     | 265/291 (91%)   | 217 (82%)  | 33 (12%)  | 15 (6%)  | 2           | 6  |
| All | All   | 3180/3492 (91%) | 2773 (87%) | 334 (10%) | 73 (2%)  | 8           | 29 |

All (73) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 67  | LEU  |
| 1   | L     | 67  | LEU  |
| 1   | L     | 138 | MET  |
| 1   | M     | 129 | THR  |
| 1   | M     | 133 | GLY  |
| 1   | C     | 66  | TYR  |
| 1   | F     | 96  | ASP  |
| 1   | F     | 229 | GLY  |
| 1   | H     | 85  | PRO  |
| 1   | J     | 33  | LEU  |
| 1   | J     | 111 | ARG  |
| 1   | J     | 157 | ALA  |
| 1   | K     | 168 | VAL  |
| 1   | L     | 66  | TYR  |
| 1   | L     | 80  | ARG  |
| 1   | L     | 253 | SER  |
| 1   | M     | 33  | LEU  |
| 1   | M     | 139 | PRO  |
| 1   | M     | 168 | VAL  |
| 1   | H     | 235 | PRO  |
| 1   | J     | 65  | ALA  |
| 1   | J     | 78  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 207 | HIS  |
| 1   | K     | 157 | ALA  |
| 1   | K     | 160 | PRO  |
| 1   | K     | 182 | ALA  |
| 1   | L     | 178 | LEU  |
| 1   | L     | 231 | GLY  |
| 1   | M     | 157 | ALA  |
| 1   | M     | 184 | VAL  |
| 1   | M     | 246 | LEU  |
| 1   | D     | 10  | PRO  |
| 1   | D     | 123 | ASP  |
| 1   | E     | 153 | GLU  |
| 1   | E     | 235 | PRO  |
| 1   | F     | 123 | ASP  |
| 1   | G     | 138 | MET  |
| 1   | I     | 103 | SER  |
| 1   | J     | 96  | ASP  |
| 1   | K     | 177 | ARG  |
| 1   | L     | 12  | ASP  |
| 1   | L     | 79  | GLU  |
| 1   | L     | 86  | GLU  |
| 1   | M     | 90  | PRO  |
| 1   | M     | 128 | GLU  |
| 1   | M     | 136 | HIS  |
| 1   | M     | 207 | HIS  |
| 1   | M     | 220 | ASP  |
| 1   | A     | 65  | ALA  |
| 1   | E     | 272 | ASN  |
| 1   | F     | 138 | MET  |
| 1   | G     | 133 | GLY  |
| 1   | I     | 157 | ALA  |
| 1   | J     | 67  | LEU  |
| 1   | K     | 110 | GLY  |
| 1   | M     | 10  | PRO  |
| 1   | M     | 138 | MET  |
| 1   | E     | 138 | MET  |
| 1   | I     | 10  | PRO  |
| 1   | I     | 139 | PRO  |
| 1   | J     | 127 | PRO  |
| 1   | K     | 267 | ILE  |
| 1   | A     | 138 | MET  |
| 1   | K     | 90  | PRO  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 102 | GLY  |
| 1   | J     | 10  | PRO  |
| 1   | C     | 138 | MET  |
| 1   | J     | 138 | MET  |
| 1   | L     | 85  | PRO  |
| 1   | D     | 138 | MET  |
| 1   | H     | 84  | LEU  |
| 1   | H     | 138 | MET  |
| 1   | I     | 138 | MET  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 218/232 (94%)   | 200 (92%)  | 18 (8%)   | 14          | 38 |
| 1   | C     | 218/232 (94%)   | 202 (93%)  | 16 (7%)   | 17          | 45 |
| 1   | D     | 218/232 (94%)   | 203 (93%)  | 15 (7%)   | 19          | 48 |
| 1   | E     | 218/232 (94%)   | 200 (92%)  | 18 (8%)   | 14          | 38 |
| 1   | F     | 218/232 (94%)   | 200 (92%)  | 18 (8%)   | 14          | 38 |
| 1   | G     | 218/232 (94%)   | 195 (89%)  | 23 (11%)  | 8           | 24 |
| 1   | H     | 218/232 (94%)   | 198 (91%)  | 20 (9%)   | 11          | 32 |
| 1   | I     | 218/232 (94%)   | 194 (89%)  | 24 (11%)  | 8           | 23 |
| 1   | J     | 218/232 (94%)   | 199 (91%)  | 19 (9%)   | 13          | 35 |
| 1   | K     | 218/232 (94%)   | 192 (88%)  | 26 (12%)  | 6           | 18 |
| 1   | L     | 218/232 (94%)   | 185 (85%)  | 33 (15%)  | 3           | 10 |
| 1   | M     | 218/232 (94%)   | 181 (83%)  | 37 (17%)  | 2           | 7  |
| All | All   | 2616/2784 (94%) | 2349 (90%) | 267 (10%) | 9           | 27 |

All (267) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | ARG  |
| 1   | A     | 37  | GLU  |
| 1   | A     | 80  | ARG  |
| 1   | A     | 109 | ARG  |
| 1   | A     | 111 | ARG  |
| 1   | A     | 153 | GLU  |
| 1   | A     | 160 | PRO  |
| 1   | A     | 161 | LYS  |
| 1   | A     | 202 | GLU  |
| 1   | A     | 206 | LYS  |
| 1   | A     | 211 | LEU  |
| 1   | A     | 225 | THR  |
| 1   | A     | 230 | VAL  |
| 1   | A     | 240 | TYR  |
| 1   | A     | 257 | GLN  |
| 1   | A     | 277 | MET  |
| 1   | A     | 291 | PHE  |
| 1   | C     | 2   | GLU  |
| 1   | C     | 42  | THR  |
| 1   | C     | 98  | SER  |
| 1   | C     | 109 | ARG  |
| 1   | C     | 111 | ARG  |
| 1   | C     | 138 | MET  |
| 1   | C     | 156 | ARG  |
| 1   | C     | 161 | LYS  |
| 1   | C     | 194 | ARG  |
| 1   | C     | 206 | LYS  |
| 1   | C     | 225 | THR  |
| 1   | C     | 232 | THR  |
| 1   | C     | 257 | GLN  |
| 1   | C     | 259 | LEU  |
| 1   | C     | 267 | ILE  |
| 1   | C     | 291 | PHE  |
| 1   | D     | 7   | VAL  |
| 1   | D     | 20  | VAL  |
| 1   | D     | 33  | LEU  |
| 1   | D     | 64  | LEU  |
| 1   | D     | 67  | LEU  |
| 1   | D     | 84  | LEU  |
| 1   | D     | 111 | ARG  |
| 1   | D     | 170 | SER  |
| 1   | D     | 199 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 211 | LEU  |
| 1   | D     | 221 | VAL  |
| 1   | D     | 255 | ARG  |
| 1   | D     | 258 | SER  |
| 1   | D     | 267 | ILE  |
| 1   | D     | 291 | PHE  |
| 1   | E     | 2   | GLU  |
| 1   | E     | 20  | VAL  |
| 1   | E     | 33  | LEU  |
| 1   | E     | 43  | VAL  |
| 1   | E     | 80  | ARG  |
| 1   | E     | 98  | SER  |
| 1   | E     | 109 | ARG  |
| 1   | E     | 144 | SER  |
| 1   | E     | 194 | ARG  |
| 1   | E     | 200 | ILE  |
| 1   | E     | 202 | GLU  |
| 1   | E     | 225 | THR  |
| 1   | E     | 226 | LEU  |
| 1   | E     | 232 | THR  |
| 1   | E     | 255 | ARG  |
| 1   | E     | 257 | GLN  |
| 1   | E     | 277 | MET  |
| 1   | E     | 291 | PHE  |
| 1   | F     | 20  | VAL  |
| 1   | F     | 33  | LEU  |
| 1   | F     | 64  | LEU  |
| 1   | F     | 67  | LEU  |
| 1   | F     | 98  | SER  |
| 1   | F     | 111 | ARG  |
| 1   | F     | 130 | SER  |
| 1   | F     | 135 | VAL  |
| 1   | F     | 138 | MET  |
| 1   | F     | 160 | PRO  |
| 1   | F     | 177 | ARG  |
| 1   | F     | 202 | GLU  |
| 1   | F     | 225 | THR  |
| 1   | F     | 226 | LEU  |
| 1   | F     | 267 | ILE  |
| 1   | F     | 273 | ARG  |
| 1   | F     | 284 | SER  |
| 1   | F     | 291 | PHE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 2   | GLU  |
| 1   | G     | 13  | LEU  |
| 1   | G     | 20  | VAL  |
| 1   | G     | 33  | LEU  |
| 1   | G     | 80  | ARG  |
| 1   | G     | 86  | GLU  |
| 1   | G     | 99  | LEU  |
| 1   | G     | 125 | ASN  |
| 1   | G     | 138 | MET  |
| 1   | G     | 144 | SER  |
| 1   | G     | 146 | LEU  |
| 1   | G     | 158 | VAL  |
| 1   | G     | 161 | LYS  |
| 1   | G     | 168 | VAL  |
| 1   | G     | 180 | LYS  |
| 1   | G     | 202 | GLU  |
| 1   | G     | 225 | THR  |
| 1   | G     | 226 | LEU  |
| 1   | G     | 232 | THR  |
| 1   | G     | 258 | SER  |
| 1   | G     | 270 | GLU  |
| 1   | G     | 289 | ARG  |
| 1   | G     | 291 | PHE  |
| 1   | H     | 2   | GLU  |
| 1   | H     | 12  | ASP  |
| 1   | H     | 33  | LEU  |
| 1   | H     | 42  | THR  |
| 1   | H     | 64  | LEU  |
| 1   | H     | 67  | LEU  |
| 1   | H     | 78  | LYS  |
| 1   | H     | 86  | GLU  |
| 1   | H     | 100 | SER  |
| 1   | H     | 109 | ARG  |
| 1   | H     | 111 | ARG  |
| 1   | H     | 146 | LEU  |
| 1   | H     | 160 | PRO  |
| 1   | H     | 175 | GLU  |
| 1   | H     | 194 | ARG  |
| 1   | H     | 206 | LYS  |
| 1   | H     | 211 | LEU  |
| 1   | H     | 225 | THR  |
| 1   | H     | 232 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 291 | PHE  |
| 1   | I     | 2   | GLU  |
| 1   | I     | 33  | LEU  |
| 1   | I     | 64  | LEU  |
| 1   | I     | 80  | ARG  |
| 1   | I     | 86  | GLU  |
| 1   | I     | 98  | SER  |
| 1   | I     | 100 | SER  |
| 1   | I     | 111 | ARG  |
| 1   | I     | 125 | ASN  |
| 1   | I     | 138 | MET  |
| 1   | I     | 144 | SER  |
| 1   | I     | 152 | THR  |
| 1   | I     | 160 | PRO  |
| 1   | I     | 161 | LYS  |
| 1   | I     | 179 | LEU  |
| 1   | I     | 194 | ARG  |
| 1   | I     | 211 | LEU  |
| 1   | I     | 221 | VAL  |
| 1   | I     | 255 | ARG  |
| 1   | I     | 267 | ILE  |
| 1   | I     | 277 | MET  |
| 1   | I     | 278 | LEU  |
| 1   | I     | 286 | LEU  |
| 1   | I     | 291 | PHE  |
| 1   | J     | 2   | GLU  |
| 1   | J     | 33  | LEU  |
| 1   | J     | 64  | LEU  |
| 1   | J     | 67  | LEU  |
| 1   | J     | 93  | LEU  |
| 1   | J     | 109 | ARG  |
| 1   | J     | 125 | ASN  |
| 1   | J     | 130 | SER  |
| 1   | J     | 140 | LEU  |
| 1   | J     | 156 | ARG  |
| 1   | J     | 158 | VAL  |
| 1   | J     | 184 | VAL  |
| 1   | J     | 194 | ARG  |
| 1   | J     | 206 | LYS  |
| 1   | J     | 225 | THR  |
| 1   | J     | 247 | MET  |
| 1   | J     | 267 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 277 | MET  |
| 1   | J     | 291 | PHE  |
| 1   | K     | 2   | GLU  |
| 1   | K     | 31  | ARG  |
| 1   | K     | 33  | LEU  |
| 1   | K     | 44  | GLU  |
| 1   | K     | 64  | LEU  |
| 1   | K     | 68  | GLU  |
| 1   | K     | 90  | PRO  |
| 1   | K     | 92  | VAL  |
| 1   | K     | 98  | SER  |
| 1   | K     | 109 | ARG  |
| 1   | K     | 113 | VAL  |
| 1   | K     | 118 | VAL  |
| 1   | K     | 126 | THR  |
| 1   | K     | 130 | SER  |
| 1   | K     | 156 | ARG  |
| 1   | K     | 160 | PRO  |
| 1   | K     | 162 | ASP  |
| 1   | K     | 194 | ARG  |
| 1   | K     | 208 | LEU  |
| 1   | K     | 216 | SER  |
| 1   | K     | 225 | THR  |
| 1   | K     | 226 | LEU  |
| 1   | K     | 230 | VAL  |
| 1   | K     | 277 | MET  |
| 1   | K     | 289 | ARG  |
| 1   | K     | 291 | PHE  |
| 1   | L     | 2   | GLU  |
| 1   | L     | 6   | VAL  |
| 1   | L     | 11  | MET  |
| 1   | L     | 33  | LEU  |
| 1   | L     | 43  | VAL  |
| 1   | L     | 51  | VAL  |
| 1   | L     | 80  | ARG  |
| 1   | L     | 85  | PRO  |
| 1   | L     | 86  | GLU  |
| 1   | L     | 88  | VAL  |
| 1   | L     | 91  | ILE  |
| 1   | L     | 98  | SER  |
| 1   | L     | 109 | ARG  |
| 1   | L     | 111 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 118 | VAL  |
| 1   | L     | 125 | ASN  |
| 1   | L     | 127 | PRO  |
| 1   | L     | 164 | VAL  |
| 1   | L     | 166 | VAL  |
| 1   | L     | 173 | PRO  |
| 1   | L     | 194 | ARG  |
| 1   | L     | 199 | ARG  |
| 1   | L     | 220 | ASP  |
| 1   | L     | 221 | VAL  |
| 1   | L     | 232 | THR  |
| 1   | L     | 257 | GLN  |
| 1   | L     | 259 | LEU  |
| 1   | L     | 260 | ASP  |
| 1   | L     | 267 | ILE  |
| 1   | L     | 268 | LEU  |
| 1   | L     | 284 | SER  |
| 1   | L     | 289 | ARG  |
| 1   | L     | 291 | PHE  |
| 1   | M     | 13  | LEU  |
| 1   | M     | 20  | VAL  |
| 1   | M     | 24  | PRO  |
| 1   | M     | 25  | SER  |
| 1   | M     | 33  | LEU  |
| 1   | M     | 39  | LEU  |
| 1   | M     | 51  | VAL  |
| 1   | M     | 64  | LEU  |
| 1   | M     | 67  | LEU  |
| 1   | M     | 68  | GLU  |
| 1   | M     | 80  | ARG  |
| 1   | M     | 84  | LEU  |
| 1   | M     | 86  | GLU  |
| 1   | M     | 90  | PRO  |
| 1   | M     | 109 | ARG  |
| 1   | M     | 111 | ARG  |
| 1   | M     | 118 | VAL  |
| 1   | M     | 129 | THR  |
| 1   | M     | 134 | ASN  |
| 1   | M     | 144 | SER  |
| 1   | M     | 150 | ARG  |
| 1   | M     | 154 | VAL  |
| 1   | M     | 160 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 168 | VAL  |
| 1   | M     | 191 | GLU  |
| 1   | M     | 192 | VAL  |
| 1   | M     | 194 | ARG  |
| 1   | M     | 200 | ILE  |
| 1   | M     | 211 | LEU  |
| 1   | M     | 232 | THR  |
| 1   | M     | 256 | VAL  |
| 1   | M     | 258 | SER  |
| 1   | M     | 260 | ASP  |
| 1   | M     | 278 | LEU  |
| 1   | M     | 284 | SER  |
| 1   | M     | 286 | LEU  |
| 1   | M     | 291 | PHE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 148 | HIS  |
| 1   | A     | 190 | HIS  |
| 1   | A     | 214 | HIS  |
| 1   | C     | 35  | GLN  |
| 1   | C     | 125 | ASN  |
| 1   | C     | 134 | ASN  |
| 1   | C     | 148 | HIS  |
| 1   | C     | 214 | HIS  |
| 1   | D     | 125 | ASN  |
| 1   | D     | 134 | ASN  |
| 1   | D     | 136 | HIS  |
| 1   | D     | 148 | HIS  |
| 1   | D     | 214 | HIS  |
| 1   | E     | 125 | ASN  |
| 1   | E     | 134 | ASN  |
| 1   | E     | 148 | HIS  |
| 1   | E     | 190 | HIS  |
| 1   | E     | 214 | HIS  |
| 1   | F     | 125 | ASN  |
| 1   | F     | 134 | ASN  |
| 1   | F     | 148 | HIS  |
| 1   | F     | 214 | HIS  |
| 1   | F     | 257 | GLN  |
| 1   | G     | 125 | ASN  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 134 | ASN  |
| 1   | G     | 148 | HIS  |
| 1   | G     | 209 | GLN  |
| 1   | G     | 214 | HIS  |
| 1   | H     | 136 | HIS  |
| 1   | H     | 148 | HIS  |
| 1   | H     | 214 | HIS  |
| 1   | I     | 125 | ASN  |
| 1   | I     | 134 | ASN  |
| 1   | I     | 148 | HIS  |
| 1   | I     | 190 | HIS  |
| 1   | I     | 214 | HIS  |
| 1   | J     | 125 | ASN  |
| 1   | J     | 134 | ASN  |
| 1   | J     | 148 | HIS  |
| 1   | J     | 214 | HIS  |
| 1   | K     | 125 | ASN  |
| 1   | K     | 134 | ASN  |
| 1   | K     | 148 | HIS  |
| 1   | K     | 190 | HIS  |
| 1   | K     | 209 | GLN  |
| 1   | K     | 214 | HIS  |
| 1   | L     | 35  | GLN  |
| 1   | L     | 125 | ASN  |
| 1   | L     | 148 | HIS  |
| 1   | L     | 190 | HIS  |
| 1   | L     | 214 | HIS  |
| 1   | M     | 125 | ASN  |
| 1   | M     | 148 | HIS  |
| 1   | M     | 190 | HIS  |
| 1   | M     | 207 | HIS  |
| 1   | M     | 214 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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     | 273/291 (93%)   | -0.11  | 4 (1%) 76 74   | 26, 42, 57, 68        | 0     |
| 1   | C     | 273/291 (93%)   | -0.09  | 2 (0%) 89 88   | 28, 48, 60, 72        | 0     |
| 1   | D     | 273/291 (93%)   | -0.01  | 8 (2%) 55 49   | 31, 45, 60, 70        | 0     |
| 1   | E     | 273/291 (93%)   | 0.06   | 8 (2%) 55 49   | 28, 48, 62, 72        | 0     |
| 1   | F     | 273/291 (93%)   | 0.03   | 2 (0%) 89 88   | 34, 47, 61, 68        | 0     |
| 1   | G     | 273/291 (93%)   | 0.12   | 9 (3%) 50 43   | 27, 53, 70, 79        | 0     |
| 1   | H     | 273/291 (93%)   | 0.03   | 4 (1%) 76 74   | 35, 55, 68, 74        | 0     |
| 1   | I     | 273/291 (93%)   | 0.01   | 6 (2%) 65 61   | 37, 56, 69, 72        | 0     |
| 1   | J     | 273/291 (93%)   | 0.11   | 5 (1%) 71 68   | 42, 60, 74, 79        | 0     |
| 1   | K     | 273/291 (93%)   | 0.68   | 48 (17%) 2 1   | 50, 68, 78, 81        | 0     |
| 1   | L     | 273/291 (93%)   | 0.63   | 31 (11%) 7 4   | 52, 67, 76, 84        | 0     |
| 1   | M     | 273/291 (93%)   | 0.99   | 61 (22%) 1 1   | 54, 73, 82, 88        | 0     |
| All | All   | 3276/3492 (93%) | 0.20   | 188 (5%) 27 22 | 26, 55, 75, 88        | 0     |

All (188) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 67  | LEU  | 8.9  |
| 1   | M     | 70  | ILE  | 6.9  |
| 1   | M     | 88  | VAL  | 6.9  |
| 1   | M     | 101 | MET  | 6.5  |
| 1   | L     | 129 | THR  | 6.0  |
| 1   | M     | 79  | GLU  | 5.7  |
| 1   | M     | 49  | VAL  | 5.4  |
| 1   | M     | 75  | LEU  | 5.4  |
| 1   | K     | 145 | GLY  | 5.4  |
| 1   | M     | 66  | TYR  | 5.3  |
| 1   | M     | 171 | LEU  | 5.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 40  | GLY  | 5.1  |
| 1   | M     | 105 | ALA  | 5.0  |
| 1   | M     | 87  | GLY  | 4.9  |
| 1   | L     | 173 | PRO  | 4.8  |
| 1   | K     | 291 | PHE  | 4.8  |
| 1   | M     | 149 | PRO  | 4.7  |
| 1   | M     | 74  | ALA  | 4.5  |
| 1   | M     | 104 | VAL  | 4.4  |
| 1   | H     | 52  | SER  | 4.4  |
| 1   | M     | 68  | GLU  | 4.4  |
| 1   | L     | 128 | GLU  | 4.3  |
| 1   | D     | 64  | LEU  | 4.3  |
| 1   | D     | 52  | SER  | 4.3  |
| 1   | H     | 113 | VAL  | 4.3  |
| 1   | M     | 186 | VAL  | 4.2  |
| 1   | M     | 52  | SER  | 4.2  |
| 1   | M     | 41  | TYR  | 4.2  |
| 1   | M     | 147 | GLY  | 4.1  |
| 1   | M     | 50  | PRO  | 4.0  |
| 1   | M     | 13  | LEU  | 4.0  |
| 1   | M     | 148 | HIS  | 4.0  |
| 1   | K     | 171 | LEU  | 3.9  |
| 1   | F     | 129 | THR  | 3.8  |
| 1   | M     | 100 | SER  | 3.8  |
| 1   | L     | 130 | SER  | 3.8  |
| 1   | M     | 128 | GLU  | 3.8  |
| 1   | L     | 50  | PRO  | 3.8  |
| 1   | G     | 134 | ASN  | 3.7  |
| 1   | A     | 64  | LEU  | 3.7  |
| 1   | G     | 66  | TYR  | 3.7  |
| 1   | L     | 127 | PRO  | 3.7  |
| 1   | M     | 154 | VAL  | 3.6  |
| 1   | M     | 129 | THR  | 3.5  |
| 1   | M     | 78  | LYS  | 3.5  |
| 1   | A     | 65  | ALA  | 3.5  |
| 1   | M     | 153 | GLU  | 3.5  |
| 1   | K     | 144 | SER  | 3.5  |
| 1   | G     | 69  | GLU  | 3.4  |
| 1   | M     | 71  | ARG  | 3.4  |
| 1   | K     | 127 | PRO  | 3.4  |
| 1   | L     | 125 | ASN  | 3.4  |
| 1   | M     | 65  | ALA  | 3.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 291 | PHE  | 3.3  |
| 1   | M     | 8   | GLY  | 3.3  |
| 1   | K     | 173 | PRO  | 3.3  |
| 1   | M     | 151 | LEU  | 3.2  |
| 1   | K     | 149 | PRO  | 3.2  |
| 1   | K     | 91  | ILE  | 3.2  |
| 1   | K     | 132 | SER  | 3.2  |
| 1   | L     | 250 | LEU  | 3.2  |
| 1   | K     | 87  | GLY  | 3.1  |
| 1   | K     | 170 | SER  | 3.1  |
| 1   | D     | 13  | LEU  | 3.1  |
| 1   | K     | 5   | ALA  | 3.1  |
| 1   | K     | 178 | LEU  | 3.0  |
| 1   | L     | 46  | LEU  | 3.0  |
| 1   | K     | 3   | ARG  | 3.0  |
| 1   | E     | 111 | ARG  | 3.0  |
| 1   | I     | 41  | TYR  | 3.0  |
| 1   | J     | 253 | SER  | 3.0  |
| 1   | G     | 127 | PRO  | 3.0  |
| 1   | I     | 286 | LEU  | 3.0  |
| 1   | K     | 85  | PRO  | 3.0  |
| 1   | M     | 9   | VAL  | 3.0  |
| 1   | E     | 66  | TYR  | 3.0  |
| 1   | D     | 133 | GLY  | 3.0  |
| 1   | L     | 181 | GLU  | 3.0  |
| 1   | M     | 170 | SER  | 3.0  |
| 1   | L     | 148 | HIS  | 2.9  |
| 1   | J     | 211 | LEU  | 2.9  |
| 1   | K     | 154 | VAL  | 2.9  |
| 1   | L     | 111 | ARG  | 2.9  |
| 1   | M     | 176 | LYS  | 2.9  |
| 1   | K     | 4   | VAL  | 2.9  |
| 1   | K     | 184 | VAL  | 2.9  |
| 1   | G     | 52  | SER  | 2.9  |
| 1   | A     | 125 | ASN  | 2.9  |
| 1   | K     | 172 | ASP  | 2.8  |
| 1   | L     | 183 | GLY  | 2.8  |
| 1   | M     | 122 | ALA  | 2.8  |
| 1   | K     | 66  | TYR  | 2.8  |
| 1   | G     | 70  | ILE  | 2.8  |
| 1   | L     | 126 | THR  | 2.8  |
| 1   | D     | 134 | ASN  | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 133 | GLY  | 2.8  |
| 1   | M     | 236 | GLY  | 2.8  |
| 1   | E     | 147 | GLY  | 2.8  |
| 1   | G     | 64  | LEU  | 2.8  |
| 1   | M     | 51  | VAL  | 2.8  |
| 1   | J     | 89  | PHE  | 2.7  |
| 1   | M     | 156 | ARG  | 2.7  |
| 1   | K     | 86  | GLU  | 2.7  |
| 1   | L     | 108 | ALA  | 2.7  |
| 1   | M     | 132 | SER  | 2.7  |
| 1   | D     | 66  | TYR  | 2.7  |
| 1   | K     | 147 | GLY  | 2.7  |
| 1   | M     | 185 | ARG  | 2.7  |
| 1   | K     | 148 | HIS  | 2.7  |
| 1   | M     | 114 | GLY  | 2.7  |
| 1   | L     | 252 | GLU  | 2.6  |
| 1   | K     | 88  | VAL  | 2.6  |
| 1   | G     | 129 | THR  | 2.6  |
| 1   | M     | 155 | PHE  | 2.6  |
| 1   | K     | 43  | VAL  | 2.6  |
| 1   | E     | 51  | VAL  | 2.6  |
| 1   | M     | 3   | ARG  | 2.6  |
| 1   | E     | 88  | VAL  | 2.6  |
| 1   | A     | 134 | ASN  | 2.6  |
| 1   | M     | 11  | MET  | 2.6  |
| 1   | C     | 64  | LEU  | 2.6  |
| 1   | K     | 125 | ASN  | 2.6  |
| 1   | L     | 186 | VAL  | 2.6  |
| 1   | K     | 65  | ALA  | 2.5  |
| 1   | M     | 271 | ARG  | 2.5  |
| 1   | M     | 130 | SER  | 2.5  |
| 1   | J     | 134 | ASN  | 2.5  |
| 1   | L     | 158 | VAL  | 2.5  |
| 1   | E     | 87  | GLY  | 2.5  |
| 1   | L     | 180 | LYS  | 2.5  |
| 1   | K     | 6   | VAL  | 2.5  |
| 1   | K     | 129 | THR  | 2.5  |
| 1   | D     | 65  | ALA  | 2.5  |
| 1   | K     | 44  | GLU  | 2.5  |
| 1   | K     | 126 | THR  | 2.5  |
| 1   | I     | 181 | GLU  | 2.5  |
| 1   | K     | 169 | ARG  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 69  | GLU  | 2.4  |
| 1   | K     | 231 | GLY  | 2.4  |
| 1   | L     | 52  | SER  | 2.4  |
| 1   | F     | 3   | ARG  | 2.4  |
| 1   | M     | 103 | SER  | 2.4  |
| 1   | H     | 65  | ALA  | 2.4  |
| 1   | L     | 134 | ASN  | 2.4  |
| 1   | K     | 134 | ASN  | 2.4  |
| 1   | M     | 180 | LYS  | 2.3  |
| 1   | M     | 46  | LEU  | 2.3  |
| 1   | K     | 2   | GLU  | 2.3  |
| 1   | L     | 286 | LEU  | 2.3  |
| 1   | M     | 12  | ASP  | 2.3  |
| 1   | M     | 136 | HIS  | 2.3  |
| 1   | I     | 231 | GLY  | 2.3  |
| 1   | E     | 154 | VAL  | 2.3  |
| 1   | E     | 13  | LEU  | 2.3  |
| 1   | L     | 176 | LYS  | 2.3  |
| 1   | M     | 83  | ALA  | 2.2  |
| 1   | K     | 128 | GLU  | 2.2  |
| 1   | K     | 92  | VAL  | 2.2  |
| 1   | M     | 172 | ASP  | 2.2  |
| 1   | M     | 133 | GLY  | 2.2  |
| 1   | H     | 13  | LEU  | 2.2  |
| 1   | K     | 42  | THR  | 2.2  |
| 1   | L     | 124 | PHE  | 2.2  |
| 1   | D     | 12  | ASP  | 2.2  |
| 1   | M     | 86  | GLU  | 2.2  |
| 1   | M     | 134 | ASN  | 2.2  |
| 1   | K     | 84  | LEU  | 2.2  |
| 1   | K     | 93  | LEU  | 2.2  |
| 1   | L     | 179 | LEU  | 2.2  |
| 1   | L     | 174 | GLY  | 2.1  |
| 1   | K     | 180 | LYS  | 2.1  |
| 1   | K     | 67  | LEU  | 2.1  |
| 1   | M     | 177 | ARG  | 2.1  |
| 1   | K     | 40  | GLY  | 2.1  |
| 1   | G     | 50  | PRO  | 2.1  |
| 1   | L     | 138 | MET  | 2.1  |
| 1   | M     | 169 | ARG  | 2.1  |
| 1   | K     | 111 | ARG  | 2.1  |
| 1   | C     | 173 | PRO  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 2   | GLU  | 2.1  |
| 1   | J     | 70  | ILE  | 2.1  |
| 1   | L     | 147 | GLY  | 2.0  |
| 1   | K     | 232 | THR  | 2.0  |
| 1   | K     | 258 | SER  | 2.0  |
| 1   | K     | 146 | LEU  | 2.0  |
| 1   | L     | 115 | VAL  | 2.0  |
| 1   | I     | 132 | SER  | 2.0  |
| 1   | K     | 82  | ALA  | 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.