



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:16 AM UTC

PDB ID : 3J8J / pdb\_00003j8j  
EMDB ID : EMD-6180  
Title : Tilted state of actin, T1  
Authors : Galkin, V.E.; Orlova, A.; Vos, M.R.; Schroder, G.F.; Egelman, E.H.  
Deposited on : 2014-11-07  
Resolution : 12.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

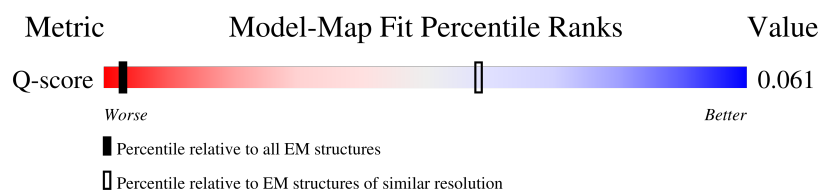
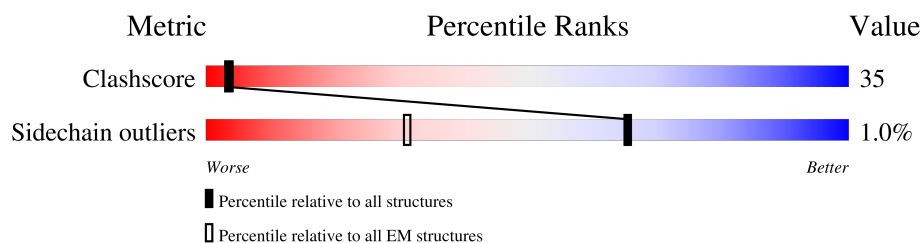
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 12.00 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.



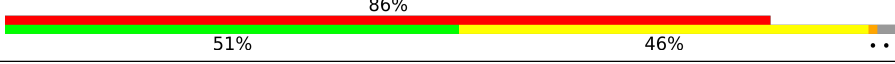
| Metric             | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|--------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore         | 229148                      | 23984                       | -                                                        |
| Sidechain outliers | 223484                      | 23102                       | -                                                        |
| Q-score            | -                           | 25397                       | 93 ( 11.50 - 12.50 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | A     | 377    | <div> <div>98%</div> <div> <div>53%</div> <div>45%</div> </div> </div> |
| 1   | B     | 377    | <div> <div>72%</div> <div> <div>51%</div> <div>46%</div> </div> </div> |
| 1   | C     | 377    | <div> <div>50%</div> <div> <div>50%</div> <div>47%</div> </div> </div> |
| 1   | D     | 377    | <div> <div>54%</div> <div> <div>50%</div> <div>48%</div> </div> </div> |
| 1   | E     | 377    | <div> <div>50%</div> <div> <div>52%</div> <div>46%</div> </div> </div> |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | F     | 377    |  |
| 1   | G     | 377    |  |
| 1   | H     | 377    |  |
| 1   | I     | 377    |  |
| 1   | J     | 377    |  |
| 1   | K     | 377    |  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31834 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

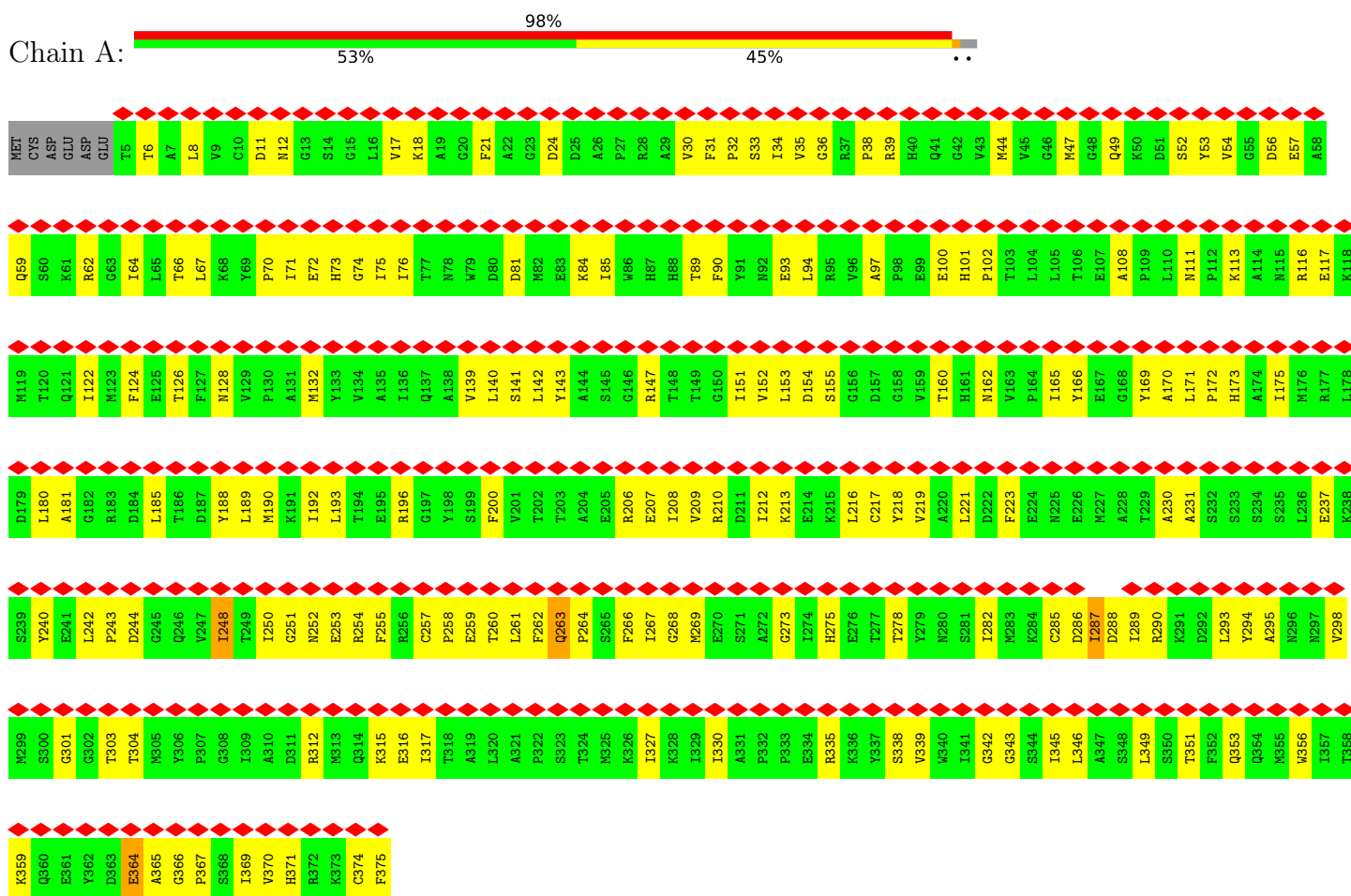
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2894  | 1833 | 487 | 553 | 21 |         |       |
| 1   | B     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2894  | 1833 | 487 | 553 | 21 |         |       |
| 1   | C     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2894  | 1833 | 487 | 553 | 21 |         |       |
| 1   | D     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2894  | 1833 | 487 | 553 | 21 |         |       |
| 1   | E     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2894  | 1833 | 487 | 553 | 21 |         |       |
| 1   | F     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2894  | 1833 | 487 | 553 | 21 |         |       |
| 1   | G     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2894  | 1833 | 487 | 553 | 21 |         |       |
| 1   | H     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2894  | 1833 | 487 | 553 | 21 |         |       |
| 1   | I     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2894  | 1833 | 487 | 553 | 21 |         |       |
| 1   | J     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2894  | 1833 | 487 | 553 | 21 |         |       |
| 1   | K     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2894  | 1833 | 487 | 553 | 21 |         |       |

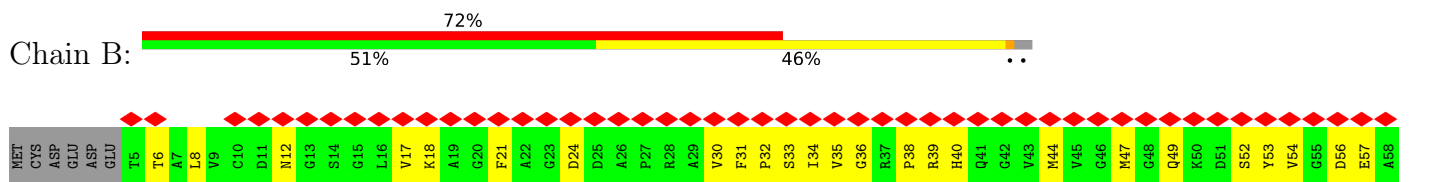
### 3 Residue-property plots

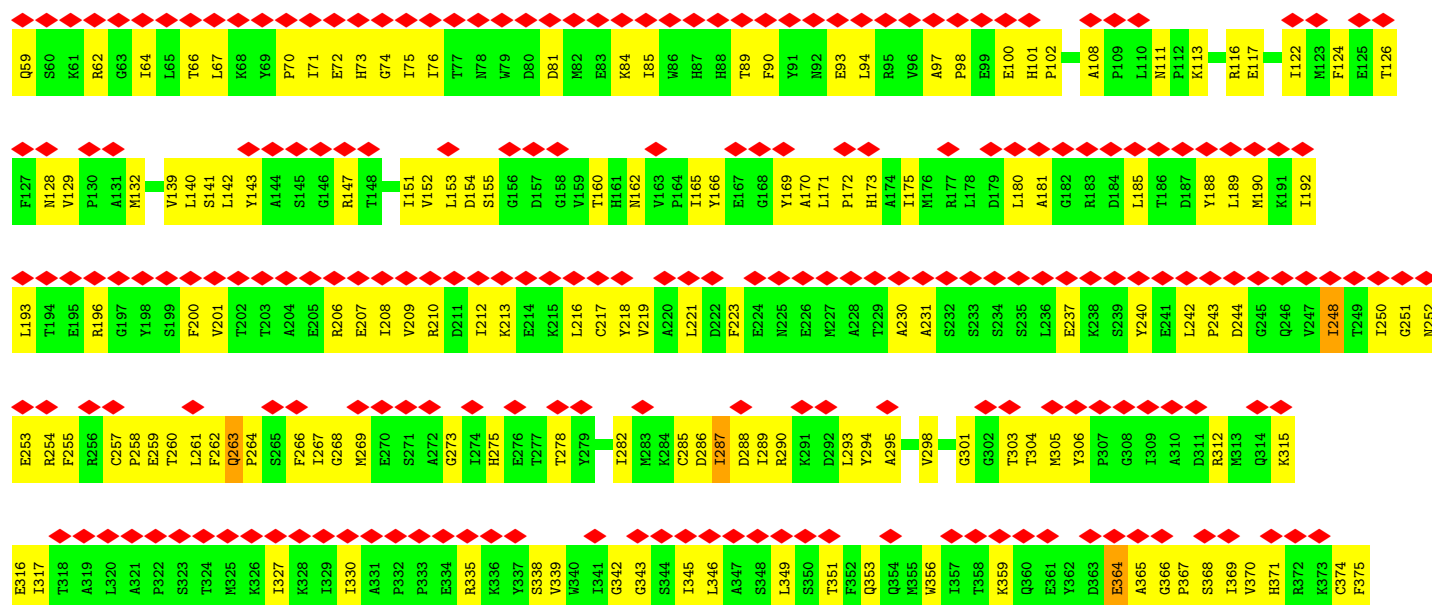
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Actin, alpha skeletal muscle

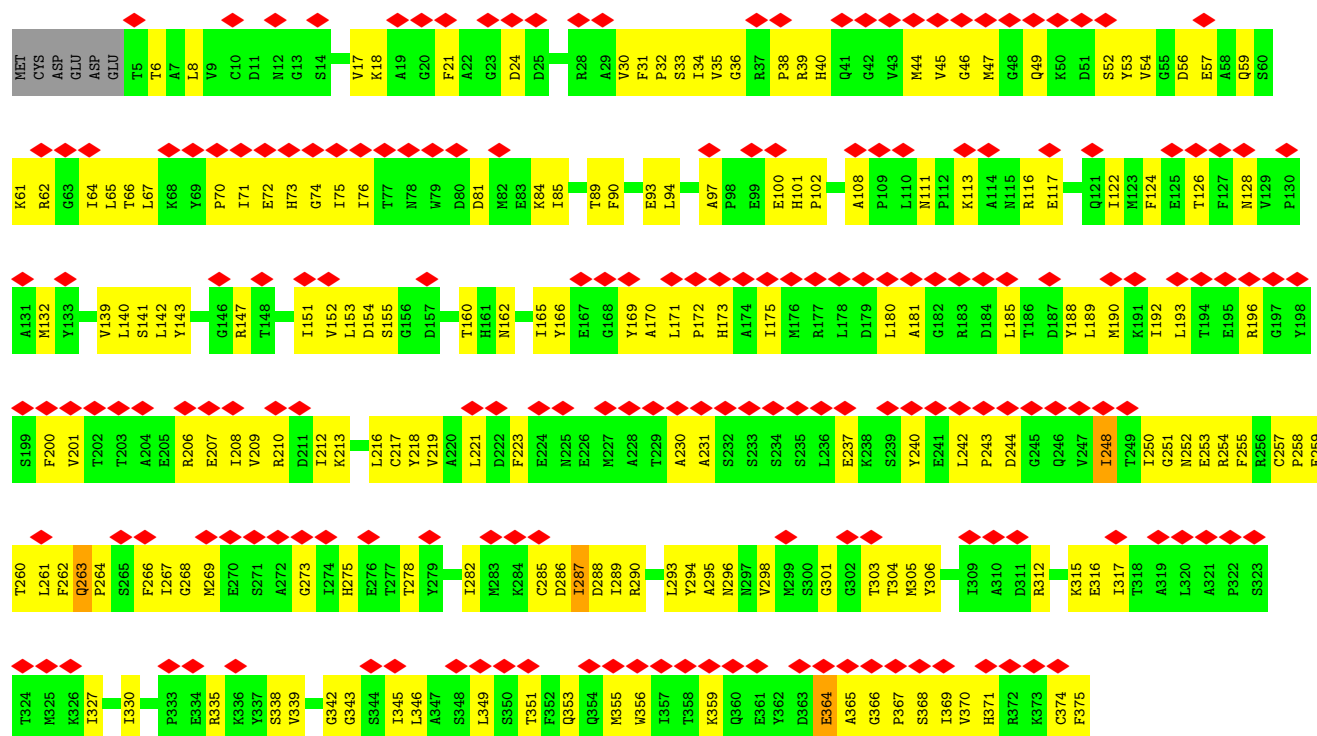


- Molecule 1: Actin, alpha skeletal muscle



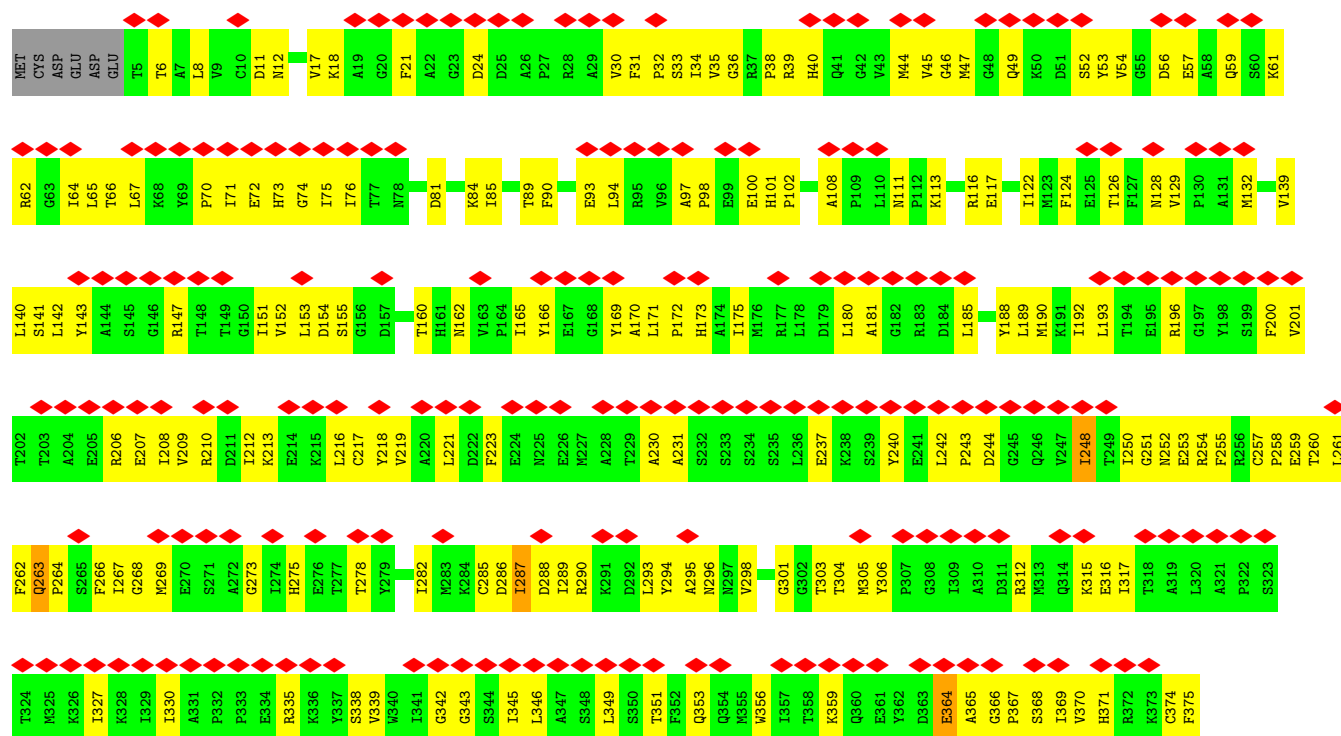


• Molecule 1: Actin, alpha skeletal muscle

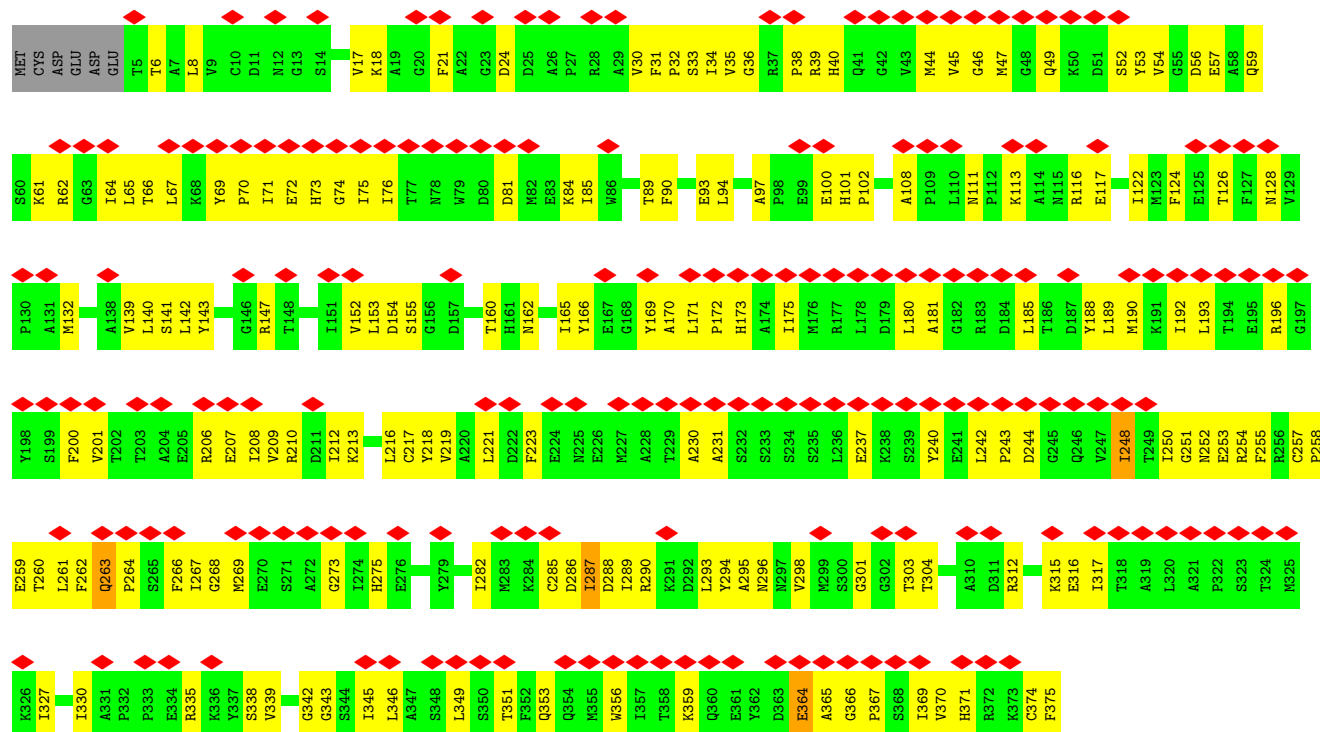


• Molecule 1: Actin, alpha skeletal muscle

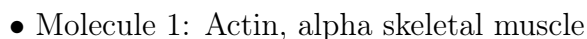




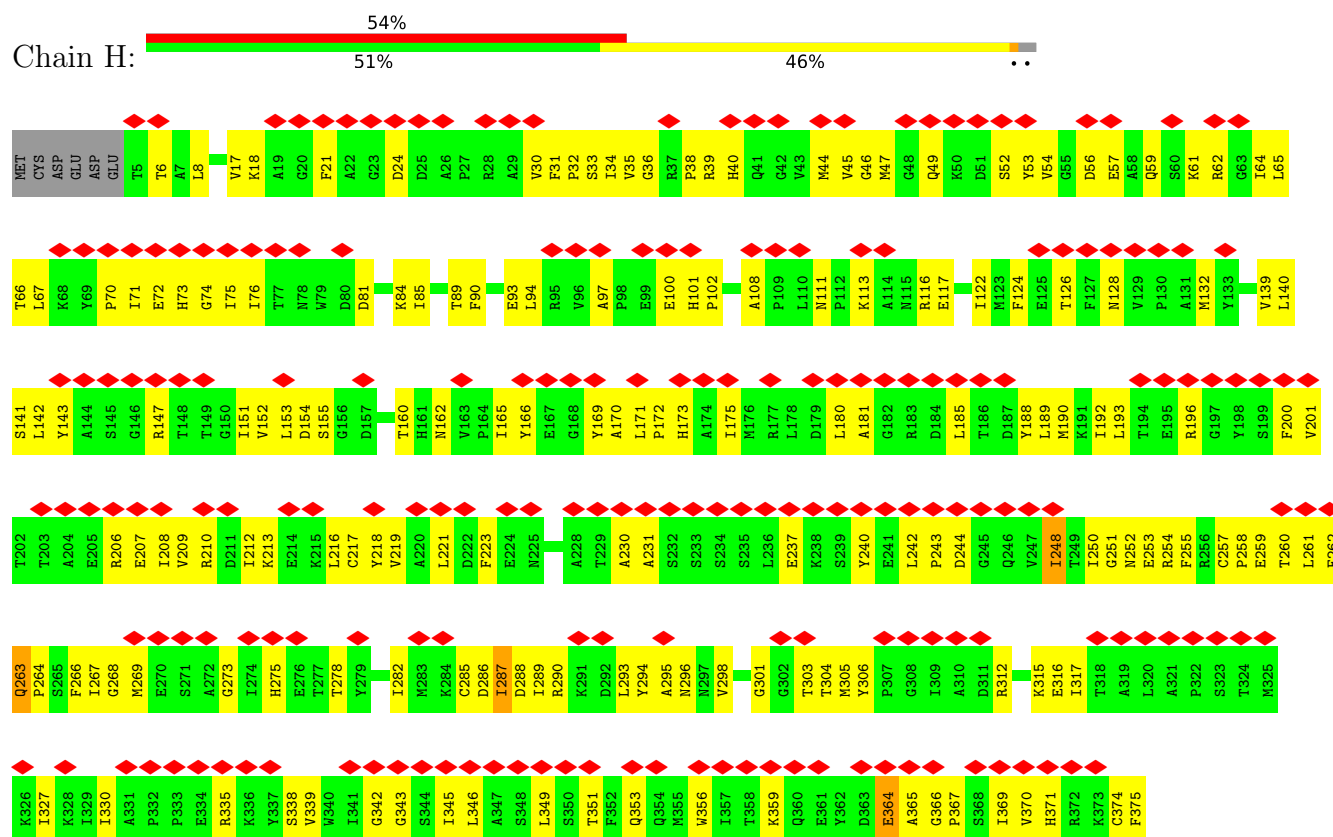
• Molecule 1: Actin, alpha skeletal muscle



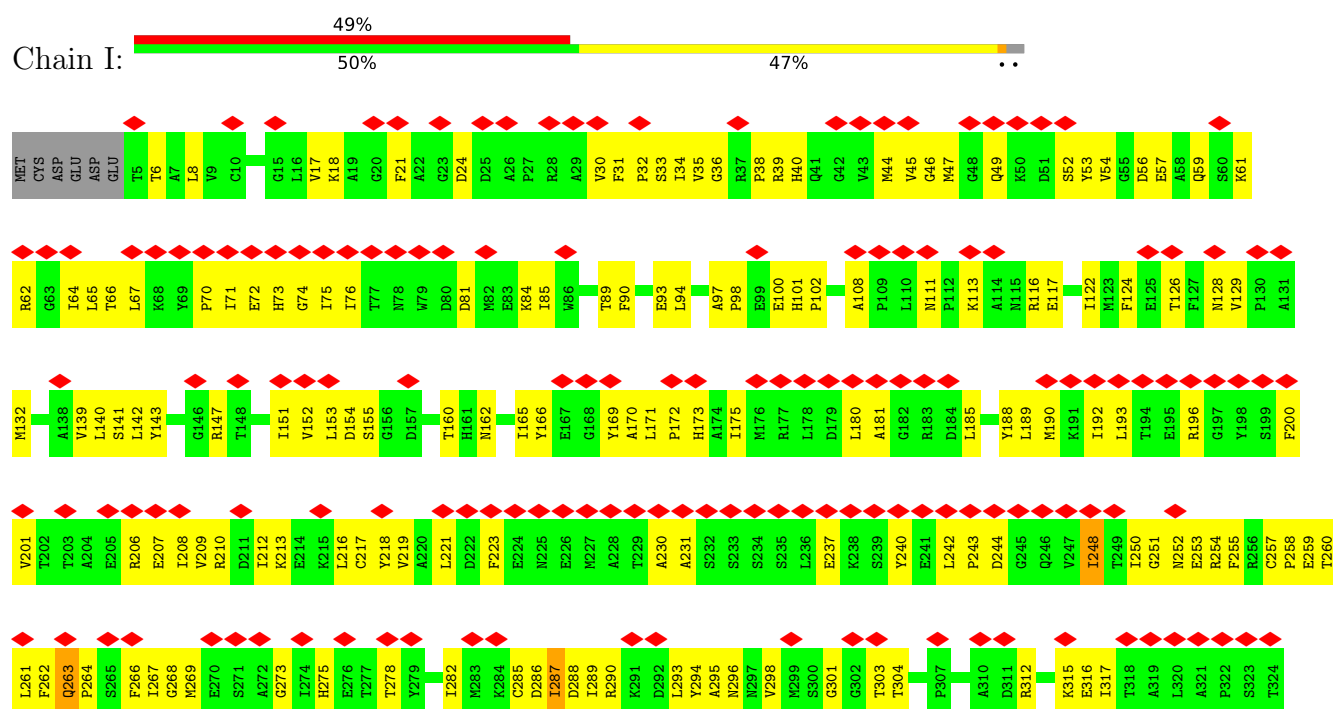
• Molecule 1: Actin, alpha skeletal muscle

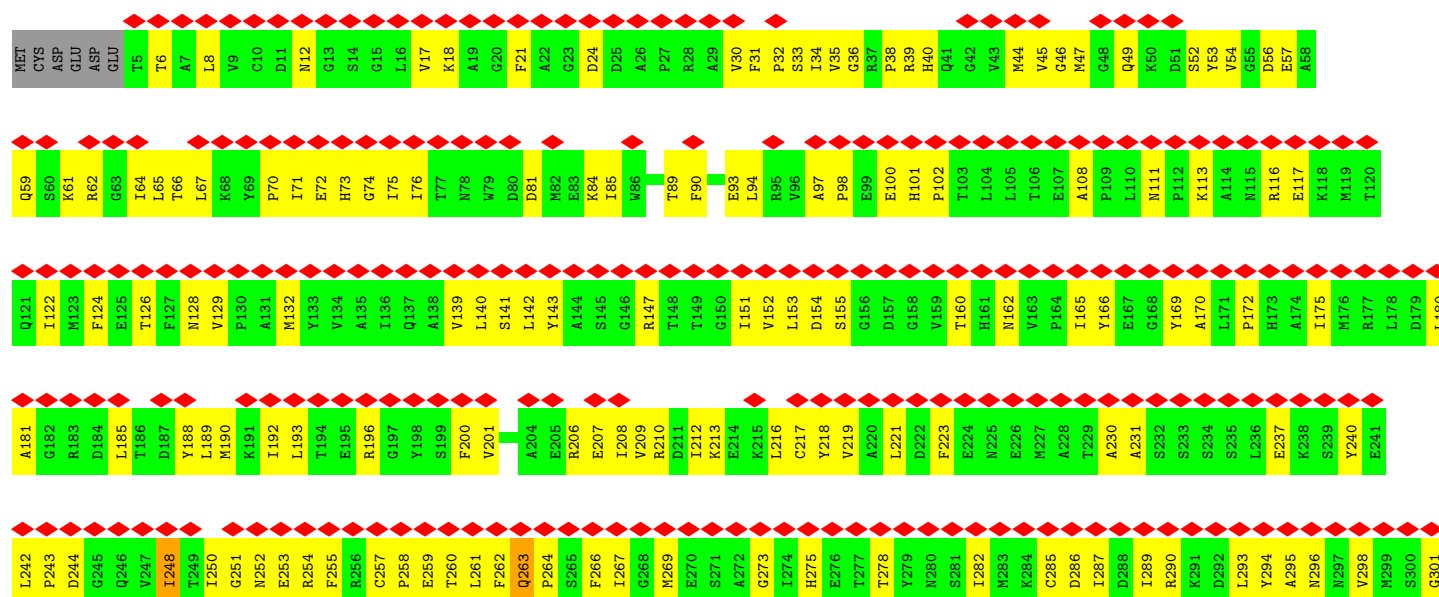


• Molecule 1: Actin, alpha skeletal muscle



• Molecule 1: Actin, alpha skeletal muscle







## 4 Experimental information

| Property                           | Value                                            | Source    |
|------------------------------------|--------------------------------------------------|-----------|
| EM reconstruction method           | HELICAL                                          | Depositor |
| Imposed symmetry                   | HELICAL, twist=166.8°, rise=28.3 Å, axial sym=C1 | Depositor |
| Number of segments used            | Not provided                                     |           |
| Resolution determination method    | FSC                                              | Depositor |
| CTF correction method              | Not provided                                     |           |
| Microscope                         | FEI TECNAI F20                                   | Depositor |
| Voltage (kV)                       | 200                                              | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | Not provided                                     |           |
| Minimum defocus (nm)               | 500                                              | Depositor |
| Maximum defocus (nm)               | 3000                                             | Depositor |
| Magnification                      | Not provided                                     |           |
| Image detector                     | KODAK SO-163 FILM                                | Depositor |
| Maximum map value                  | 0.117                                            | Depositor |
| Minimum map value                  | -0.051                                           | Depositor |
| Average map value                  | 0.001                                            | Depositor |
| Map value standard deviation       | 0.014                                            | Depositor |
| Recommended contour level          | 0.07                                             | Depositor |
| Map size (Å)                       | 250.0, 250.0, 250.0                              | wwPDB     |
| Map dimensions                     | 100, 100, 100                                    | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0                                 | wwPDB     |
| Pixel spacing (Å)                  | 2.5, 2.5, 2.5                                    | Depositor |

## 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     | 0.61         | 0/2956      | 0.94        | 4/4004 (0.1%)   |
| 1   | B     | 0.61         | 0/2956      | 0.94        | 4/4004 (0.1%)   |
| 1   | C     | 0.61         | 0/2956      | 0.94        | 4/4004 (0.1%)   |
| 1   | D     | 0.61         | 0/2956      | 0.95        | 4/4004 (0.1%)   |
| 1   | E     | 0.61         | 0/2956      | 0.95        | 4/4004 (0.1%)   |
| 1   | F     | 0.61         | 0/2956      | 0.94        | 4/4004 (0.1%)   |
| 1   | G     | 0.61         | 0/2956      | 0.94        | 4/4004 (0.1%)   |
| 1   | H     | 0.61         | 0/2956      | 0.95        | 4/4004 (0.1%)   |
| 1   | I     | 0.61         | 0/2956      | 0.94        | 4/4004 (0.1%)   |
| 1   | J     | 0.61         | 0/2956      | 0.95        | 4/4004 (0.1%)   |
| 1   | K     | 0.61         | 0/2956      | 0.95        | 4/4004 (0.1%)   |
| All | All   | 0.61         | 0/32516     | 0.94        | 44/44044 (0.1%) |

There are no bond length outliers.

All (44) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|------|------------------------|---------------------|
| 1   | G     | 287 | ILE  | N-CA-C | 5.76 | 116.49                 | 110.62              |
| 1   | C     | 287 | ILE  | N-CA-C | 5.75 | 116.48                 | 110.62              |
| 1   | I     | 287 | ILE  | N-CA-C | 5.73 | 116.46                 | 110.62              |
| 1   | J     | 62  | ARG  | N-CA-C | 5.73 | 117.52                 | 111.28              |
| 1   | H     | 62  | ARG  | N-CA-C | 5.72 | 117.52                 | 111.28              |
| 1   | B     | 287 | ILE  | N-CA-C | 5.71 | 116.44                 | 110.62              |
| 1   | H     | 287 | ILE  | N-CA-C | 5.71 | 116.44                 | 110.62              |
| 1   | K     | 62  | ARG  | N-CA-C | 5.70 | 117.50                 | 111.28              |
| 1   | B     | 62  | ARG  | N-CA-C | 5.70 | 117.49                 | 111.28              |
| 1   | J     | 287 | ILE  | N-CA-C | 5.70 | 116.44                 | 110.62              |
| 1   | C     | 62  | ARG  | N-CA-C | 5.70 | 117.49                 | 111.28              |
| 1   | D     | 287 | ILE  | N-CA-C | 5.70 | 116.43                 | 110.62              |
| 1   | D     | 62  | ARG  | N-CA-C | 5.69 | 117.48                 | 111.28              |
| 1   | E     | 287 | ILE  | N-CA-C | 5.68 | 116.41                 | 110.62              |
| 1   | F     | 287 | ILE  | N-CA-C | 5.67 | 116.40                 | 110.62              |
| 1   | I     | 62  | ARG  | N-CA-C | 5.67 | 117.46                 | 111.28              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | A     | 287 | ILE  | N-CA-C | 5.67 | 116.40      | 110.62   |
| 1   | E     | 62  | ARG  | N-CA-C | 5.67 | 117.46      | 111.28   |
| 1   | A     | 62  | ARG  | N-CA-C | 5.67 | 117.45      | 111.28   |
| 1   | G     | 62  | ARG  | N-CA-C | 5.66 | 117.45      | 111.28   |
| 1   | K     | 287 | ILE  | N-CA-C | 5.65 | 116.39      | 110.62   |
| 1   | F     | 62  | ARG  | N-CA-C | 5.65 | 117.44      | 111.28   |
| 1   | A     | 263 | GLN  | CA-C-N | 5.18 | 124.84      | 119.56   |
| 1   | A     | 263 | GLN  | C-N-CA | 5.18 | 124.84      | 119.56   |
| 1   | B     | 263 | GLN  | CA-C-N | 5.18 | 124.84      | 119.56   |
| 1   | B     | 263 | GLN  | C-N-CA | 5.18 | 124.84      | 119.56   |
| 1   | E     | 263 | GLN  | CA-C-N | 5.17 | 124.83      | 119.56   |
| 1   | E     | 263 | GLN  | C-N-CA | 5.17 | 124.83      | 119.56   |
| 1   | J     | 263 | GLN  | CA-C-N | 5.17 | 124.83      | 119.56   |
| 1   | J     | 263 | GLN  | C-N-CA | 5.17 | 124.83      | 119.56   |
| 1   | G     | 263 | GLN  | CA-C-N | 5.14 | 124.81      | 119.56   |
| 1   | G     | 263 | GLN  | C-N-CA | 5.14 | 124.81      | 119.56   |
| 1   | I     | 263 | GLN  | CA-C-N | 5.14 | 124.81      | 119.56   |
| 1   | I     | 263 | GLN  | C-N-CA | 5.14 | 124.81      | 119.56   |
| 1   | F     | 263 | GLN  | CA-C-N | 5.13 | 124.80      | 119.56   |
| 1   | F     | 263 | GLN  | C-N-CA | 5.13 | 124.80      | 119.56   |
| 1   | C     | 263 | GLN  | CA-C-N | 5.12 | 124.78      | 119.56   |
| 1   | C     | 263 | GLN  | C-N-CA | 5.12 | 124.78      | 119.56   |
| 1   | K     | 263 | GLN  | CA-C-N | 5.12 | 124.78      | 119.56   |
| 1   | K     | 263 | GLN  | C-N-CA | 5.12 | 124.78      | 119.56   |
| 1   | H     | 263 | GLN  | CA-C-N | 5.11 | 124.78      | 119.56   |
| 1   | H     | 263 | GLN  | C-N-CA | 5.11 | 124.78      | 119.56   |
| 1   | D     | 263 | GLN  | CA-C-N | 5.11 | 124.77      | 119.56   |
| 1   | D     | 263 | GLN  | C-N-CA | 5.11 | 124.77      | 119.56   |

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     | 2894  | 0        | 2866     | 208     | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 2894  | 0        | 2866     | 214     | 0            |
| 1   | C     | 2894  | 0        | 2866     | 270     | 0            |
| 1   | D     | 2894  | 0        | 2866     | 270     | 0            |
| 1   | E     | 2894  | 0        | 2866     | 265     | 0            |
| 1   | F     | 2894  | 0        | 2866     | 269     | 0            |
| 1   | G     | 2894  | 0        | 2866     | 270     | 0            |
| 1   | H     | 2894  | 0        | 2866     | 269     | 0            |
| 1   | I     | 2894  | 0        | 2866     | 270     | 0            |
| 1   | J     | 2894  | 0        | 2866     | 218     | 0            |
| 1   | K     | 2894  | 0        | 2866     | 214     | 0            |
| All | All   | 31834 | 0        | 31526    | 2224    | 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 35.

All (2224) 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:I:171:LEU:CD2  | 1:K:45:VAL:HG12 | 1.60                     | 1.31              |
| 1:D:171:LEU:CD2  | 1:F:45:VAL:HG12 | 1.60                     | 1.31              |
| 1:C:171:LEU:CD2  | 1:E:45:VAL:HG12 | 1.60                     | 1.30              |
| 1:G:171:LEU:CD2  | 1:I:45:VAL:HG12 | 1.61                     | 1.30              |
| 1:E:171:LEU:CD2  | 1:G:45:VAL:HG12 | 1.61                     | 1.29              |
| 1:B:171:LEU:CD2  | 1:D:45:VAL:HG12 | 1.61                     | 1.29              |
| 1:F:171:LEU:CD2  | 1:H:45:VAL:HG12 | 1.61                     | 1.28              |
| 1:A:171:LEU:CD2  | 1:C:45:VAL:HG12 | 1.60                     | 1.28              |
| 1:H:171:LEU:CD2  | 1:J:45:VAL:HG12 | 1.61                     | 1.28              |
| 1:C:171:LEU:HD22 | 1:E:45:VAL:CG1  | 1.66                     | 1.26              |
| 1:E:171:LEU:HD22 | 1:G:45:VAL:CG1  | 1.66                     | 1.25              |
| 1:B:171:LEU:HD22 | 1:D:45:VAL:CG1  | 1.66                     | 1.25              |
| 1:A:171:LEU:HD22 | 1:C:45:VAL:CG1  | 1.66                     | 1.25              |
| 1:G:171:LEU:HD22 | 1:I:45:VAL:CG1  | 1.66                     | 1.25              |
| 1:H:171:LEU:HD22 | 1:J:45:VAL:CG1  | 1.66                     | 1.24              |
| 1:D:171:LEU:HD22 | 1:F:45:VAL:CG1  | 1.66                     | 1.24              |
| 1:I:171:LEU:HD22 | 1:K:45:VAL:CG1  | 1.66                     | 1.24              |
| 1:F:171:LEU:HD22 | 1:H:45:VAL:CG1  | 1.66                     | 1.23              |
| 1:F:290:ARG:CD   | 1:H:64:ILE:HD11 | 1.71                     | 1.21              |
| 1:D:290:ARG:CD   | 1:F:64:ILE:HD11 | 1.71                     | 1.20              |
| 1:B:290:ARG:CD   | 1:D:64:ILE:HD11 | 1.71                     | 1.20              |
| 1:I:290:ARG:CD   | 1:K:64:ILE:HD11 | 1.71                     | 1.20              |
| 1:C:290:ARG:CD   | 1:E:64:ILE:HD11 | 1.71                     | 1.19              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:290:ARG:CD  | 1:J:64:ILE:HD11 | 1.71                     | 1.19              |
| 1:A:290:ARG:CD  | 1:C:64:ILE:HD11 | 1.71                     | 1.19              |
| 1:E:290:ARG:CD  | 1:G:64:ILE:HD11 | 1.71                     | 1.19              |
| 1:G:290:ARG:CD  | 1:I:64:ILE:HD11 | 1.71                     | 1.19              |
| 1:E:286:ASP:OD1 | 1:G:47:MET:HA   | 1.45                     | 1.16              |
| 1:G:286:ASP:OD1 | 1:I:47:MET:HA   | 1.45                     | 1.16              |
| 1:I:286:ASP:OD1 | 1:K:47:MET:HA   | 1.45                     | 1.16              |
| 1:B:290:ARG:HD2 | 1:D:64:ILE:CD1  | 1.77                     | 1.15              |
| 1:E:290:ARG:HD2 | 1:G:64:ILE:CD1  | 1.77                     | 1.15              |
| 1:B:286:ASP:OD1 | 1:D:47:MET:HA   | 1.45                     | 1.15              |
| 1:D:290:ARG:HD2 | 1:F:64:ILE:CD1  | 1.77                     | 1.15              |
| 1:C:290:ARG:HD2 | 1:E:64:ILE:CD1  | 1.77                     | 1.14              |
| 1:G:290:ARG:HD2 | 1:I:64:ILE:CD1  | 1.77                     | 1.14              |
| 1:I:290:ARG:HD2 | 1:K:64:ILE:CD1  | 1.77                     | 1.14              |
| 1:A:286:ASP:OD1 | 1:C:47:MET:HA   | 1.45                     | 1.13              |
| 1:F:290:ARG:HD2 | 1:H:64:ILE:CD1  | 1.77                     | 1.13              |
| 1:D:286:ASP:OD1 | 1:F:47:MET:HA   | 1.45                     | 1.13              |
| 1:F:74:GLY:O    | 1:F:75:ILE:HG13 | 1.49                     | 1.13              |
| 1:H:74:GLY:O    | 1:H:75:ILE:HG13 | 1.49                     | 1.13              |
| 1:E:74:GLY:O    | 1:E:75:ILE:HG13 | 1.49                     | 1.13              |
| 1:G:74:GLY:O    | 1:G:75:ILE:HG13 | 1.49                     | 1.13              |
| 1:J:74:GLY:O    | 1:J:75:ILE:HG13 | 1.49                     | 1.13              |
| 1:A:290:ARG:HD2 | 1:C:64:ILE:CD1  | 1.77                     | 1.13              |
| 1:C:74:GLY:O    | 1:C:75:ILE:HG13 | 1.49                     | 1.13              |
| 1:A:74:GLY:O    | 1:A:75:ILE:HG13 | 1.49                     | 1.12              |
| 1:D:74:GLY:O    | 1:D:75:ILE:HG13 | 1.49                     | 1.12              |
| 1:I:74:GLY:O    | 1:I:75:ILE:HG13 | 1.49                     | 1.13              |
| 1:B:74:GLY:O    | 1:B:75:ILE:HG13 | 1.49                     | 1.12              |
| 1:K:74:GLY:O    | 1:K:75:ILE:HG13 | 1.49                     | 1.12              |
| 1:C:286:ASP:OD1 | 1:E:47:MET:HA   | 1.45                     | 1.12              |
| 1:H:290:ARG:HD2 | 1:J:64:ILE:CD1  | 1.77                     | 1.12              |
| 1:H:286:ASP:OD1 | 1:J:47:MET:HA   | 1.45                     | 1.11              |
| 1:F:286:ASP:OD1 | 1:H:47:MET:HA   | 1.45                     | 1.10              |
| 1:G:290:ARG:NH1 | 1:I:64:ILE:HG12 | 1.69                     | 1.07              |
| 1:A:173:HIS:HE1 | 1:C:45:VAL:HG11 | 1.20                     | 1.07              |
| 1:H:290:ARG:NH1 | 1:J:64:ILE:HG12 | 1.69                     | 1.07              |
| 1:D:290:ARG:NH1 | 1:F:64:ILE:HG12 | 1.69                     | 1.06              |
| 1:H:173:HIS:HE1 | 1:J:45:VAL:HG11 | 1.20                     | 1.06              |
| 1:I:290:ARG:NH1 | 1:K:64:ILE:HG12 | 1.69                     | 1.06              |
| 1:C:290:ARG:NH1 | 1:E:64:ILE:HG12 | 1.69                     | 1.06              |
| 1:E:290:ARG:NH1 | 1:G:64:ILE:HG12 | 1.69                     | 1.06              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:290:ARG:NH1  | 1:C:64:ILE:HG12 | 1.69                     | 1.06              |
| 1:B:290:ARG:NH1  | 1:D:64:ILE:HG12 | 1.69                     | 1.06              |
| 1:C:173:HIS:HE1  | 1:E:45:VAL:HG11 | 1.20                     | 1.06              |
| 1:F:173:HIS:HE1  | 1:H:45:VAL:HG11 | 1.20                     | 1.06              |
| 1:F:290:ARG:NH1  | 1:H:64:ILE:HG12 | 1.69                     | 1.06              |
| 1:D:173:HIS:HE1  | 1:F:45:VAL:HG11 | 1.20                     | 1.04              |
| 1:E:173:HIS:HE1  | 1:G:45:VAL:HG11 | 1.20                     | 1.04              |
| 1:I:173:HIS:HE1  | 1:K:45:VAL:HG11 | 1.20                     | 1.03              |
| 1:G:171:LEU:HD22 | 1:I:45:VAL:HG12 | 1.03                     | 1.03              |
| 1:C:171:LEU:HD22 | 1:E:45:VAL:HG12 | 1.03                     | 1.03              |
| 1:I:171:LEU:HD22 | 1:K:45:VAL:HG12 | 1.03                     | 1.03              |
| 1:A:171:LEU:HD22 | 1:C:45:VAL:HG12 | 1.03                     | 1.02              |
| 1:G:173:HIS:HE1  | 1:I:45:VAL:HG11 | 1.20                     | 1.02              |
| 1:B:173:HIS:HE1  | 1:D:45:VAL:HG11 | 1.20                     | 1.02              |
| 1:B:171:LEU:HD22 | 1:D:45:VAL:HG12 | 1.03                     | 1.01              |
| 1:A:290:ARG:CZ   | 1:C:64:ILE:HG12 | 1.90                     | 1.01              |
| 1:B:290:ARG:CZ   | 1:D:64:ILE:HG12 | 1.90                     | 1.01              |
| 1:E:290:ARG:CZ   | 1:G:64:ILE:HG12 | 1.91                     | 1.01              |
| 1:H:290:ARG:CZ   | 1:J:64:ILE:HG12 | 1.91                     | 1.01              |
| 1:D:171:LEU:HD22 | 1:F:45:VAL:HG12 | 1.03                     | 1.01              |
| 1:H:171:LEU:HD22 | 1:J:45:VAL:HG12 | 1.03                     | 1.01              |
| 1:F:290:ARG:CZ   | 1:H:64:ILE:HG12 | 1.90                     | 1.01              |
| 1:G:290:ARG:CZ   | 1:I:64:ILE:HG12 | 1.90                     | 1.01              |
| 1:D:290:ARG:CZ   | 1:F:64:ILE:HG12 | 1.90                     | 1.01              |
| 1:C:290:ARG:CZ   | 1:E:64:ILE:HG12 | 1.90                     | 1.00              |
| 1:I:290:ARG:CZ   | 1:K:64:ILE:HG12 | 1.90                     | 1.00              |
| 1:E:73:HIS:CB    | 1:E:74:GLY:HA3  | 1.90                     | 1.00              |
| 1:E:171:LEU:HD22 | 1:G:45:VAL:HG12 | 1.03                     | 1.00              |
| 1:G:73:HIS:CB    | 1:G:74:GLY:HA3  | 1.90                     | 1.00              |
| 1:A:173:HIS:CE1  | 1:C:45:VAL:HG11 | 1.96                     | 1.00              |
| 1:I:73:HIS:CB    | 1:I:74:GLY:HA3  | 1.90                     | 1.00              |
| 1:D:173:HIS:CE1  | 1:F:45:VAL:HG11 | 1.96                     | 1.00              |
| 1:B:173:HIS:CE1  | 1:D:45:VAL:HG11 | 1.96                     | 0.99              |
| 1:D:73:HIS:CB    | 1:D:74:GLY:HA3  | 1.90                     | 0.99              |
| 1:C:173:HIS:CE1  | 1:E:45:VAL:HG11 | 1.96                     | 0.99              |
| 1:K:73:HIS:CB    | 1:K:74:GLY:HA3  | 1.90                     | 0.99              |
| 1:C:73:HIS:CB    | 1:C:74:GLY:HA3  | 1.90                     | 0.99              |
| 1:F:171:LEU:HD22 | 1:H:45:VAL:HG12 | 1.03                     | 0.99              |
| 1:F:173:HIS:CE1  | 1:H:45:VAL:HG11 | 1.96                     | 0.99              |
| 1:I:173:HIS:CE1  | 1:K:45:VAL:HG11 | 1.96                     | 0.99              |
| 1:E:173:HIS:CE1  | 1:G:45:VAL:HG11 | 1.96                     | 0.99              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:173:HIS:CE1  | 1:I:45:VAL:HG11 | 1.96                     | 0.99              |
| 1:H:173:HIS:CE1  | 1:J:45:VAL:HG11 | 1.96                     | 0.98              |
| 1:J:73:HIS:CB    | 1:J:74:GLY:HA3  | 1.90                     | 0.98              |
| 1:B:73:HIS:CB    | 1:B:74:GLY:HA3  | 1.90                     | 0.98              |
| 1:A:73:HIS:CB    | 1:A:74:GLY:HA3  | 1.90                     | 0.98              |
| 1:H:73:HIS:CB    | 1:H:74:GLY:HA3  | 1.90                     | 0.97              |
| 1:F:73:HIS:CB    | 1:F:74:GLY:HA3  | 1.90                     | 0.96              |
| 1:E:290:ARG:CD   | 1:G:64:ILE:CD1  | 2.43                     | 0.91              |
| 1:I:290:ARG:CD   | 1:K:64:ILE:CD1  | 2.43                     | 0.91              |
| 1:A:290:ARG:CD   | 1:C:64:ILE:CD1  | 2.43                     | 0.91              |
| 1:F:290:ARG:HD2  | 1:H:64:ILE:HD11 | 0.90                     | 0.90              |
| 1:E:290:ARG:HD2  | 1:G:64:ILE:HD11 | 0.90                     | 0.90              |
| 1:C:290:ARG:HD2  | 1:E:64:ILE:HD11 | 0.90                     | 0.90              |
| 1:D:290:ARG:HD2  | 1:F:64:ILE:HD11 | 0.90                     | 0.90              |
| 1:G:73:HIS:CB    | 1:G:74:GLY:CA   | 2.50                     | 0.90              |
| 1:I:73:HIS:CB    | 1:I:74:GLY:CA   | 2.50                     | 0.90              |
| 1:A:290:ARG:HD2  | 1:C:64:ILE:HD11 | 0.90                     | 0.89              |
| 1:G:290:ARG:HD2  | 1:I:64:ILE:HD11 | 0.90                     | 0.89              |
| 1:B:290:ARG:HD2  | 1:D:64:ILE:HD11 | 0.90                     | 0.89              |
| 1:I:290:ARG:HD2  | 1:K:64:ILE:HD11 | 0.90                     | 0.89              |
| 1:A:73:HIS:CB    | 1:A:74:GLY:CA   | 2.50                     | 0.89              |
| 1:E:73:HIS:CB    | 1:E:74:GLY:CA   | 2.50                     | 0.89              |
| 1:J:73:HIS:CB    | 1:J:74:GLY:CA   | 2.50                     | 0.89              |
| 1:H:73:HIS:CB    | 1:H:74:GLY:CA   | 2.50                     | 0.89              |
| 1:K:73:HIS:CB    | 1:K:74:GLY:CA   | 2.50                     | 0.88              |
| 1:D:73:HIS:CB    | 1:D:74:GLY:CA   | 2.50                     | 0.88              |
| 1:F:73:HIS:CB    | 1:F:74:GLY:CA   | 2.50                     | 0.88              |
| 1:B:290:ARG:CD   | 1:D:64:ILE:CD1  | 2.43                     | 0.88              |
| 1:H:290:ARG:CD   | 1:J:64:ILE:CD1  | 2.43                     | 0.88              |
| 1:D:290:ARG:CD   | 1:F:64:ILE:CD1  | 2.43                     | 0.87              |
| 1:B:73:HIS:CB    | 1:B:74:GLY:CA   | 2.50                     | 0.87              |
| 1:H:290:ARG:HD2  | 1:J:64:ILE:HD11 | 0.90                     | 0.87              |
| 1:G:290:ARG:CD   | 1:I:64:ILE:CD1  | 2.43                     | 0.86              |
| 1:C:290:ARG:CD   | 1:E:64:ILE:CD1  | 2.43                     | 0.86              |
| 1:C:73:HIS:CB    | 1:C:74:GLY:CA   | 2.50                     | 0.86              |
| 1:A:286:ASP:OD1  | 1:C:47:MET:CA   | 2.24                     | 0.86              |
| 1:D:286:ASP:OD1  | 1:F:47:MET:CA   | 2.24                     | 0.86              |
| 1:F:290:ARG:CD   | 1:H:64:ILE:CD1  | 2.43                     | 0.86              |
| 1:G:287:ILE:HG12 | 1:I:65:LEU:HG   | 1.58                     | 0.86              |
| 1:H:286:ASP:OD1  | 1:J:47:MET:CA   | 2.24                     | 0.86              |
| 1:A:74:GLY:O     | 1:A:75:ILE:CG1  | 2.24                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:287:ILE:HG12 | 1:D:65:LEU:HG   | 1.58                     | 0.86              |
| 1:E:287:ILE:HG12 | 1:G:65:LEU:HG   | 1.58                     | 0.86              |
| 1:H:74:GLY:O     | 1:H:75:ILE:CG1  | 2.24                     | 0.86              |
| 1:E:74:GLY:O     | 1:E:75:ILE:CG1  | 2.24                     | 0.86              |
| 1:E:286:ASP:OD1  | 1:G:47:MET:CA   | 2.24                     | 0.86              |
| 1:J:74:GLY:O     | 1:J:75:ILE:CG1  | 2.24                     | 0.85              |
| 1:D:74:GLY:O     | 1:D:75:ILE:CG1  | 2.24                     | 0.85              |
| 1:I:287:ILE:HG12 | 1:K:65:LEU:HG   | 1.58                     | 0.85              |
| 1:G:74:GLY:O     | 1:G:75:ILE:CG1  | 2.24                     | 0.85              |
| 1:I:286:ASP:OD1  | 1:K:47:MET:CA   | 2.24                     | 0.85              |
| 1:C:74:GLY:O     | 1:C:75:ILE:CG1  | 2.24                     | 0.85              |
| 1:C:286:ASP:OD1  | 1:E:47:MET:CA   | 2.24                     | 0.85              |
| 1:F:286:ASP:OD1  | 1:H:47:MET:CA   | 2.24                     | 0.85              |
| 1:K:74:GLY:O     | 1:K:75:ILE:CG1  | 2.24                     | 0.85              |
| 1:D:287:ILE:HG12 | 1:F:65:LEU:HG   | 1.58                     | 0.85              |
| 1:B:286:ASP:OD1  | 1:D:47:MET:CA   | 2.24                     | 0.85              |
| 1:F:74:GLY:O     | 1:F:75:ILE:CG1  | 2.24                     | 0.85              |
| 1:A:287:ILE:HG12 | 1:C:65:LEU:HG   | 1.58                     | 0.85              |
| 1:I:74:GLY:O     | 1:I:75:ILE:CG1  | 2.24                     | 0.85              |
| 1:C:287:ILE:HG12 | 1:E:65:LEU:HG   | 1.58                     | 0.84              |
| 1:G:286:ASP:OD1  | 1:I:47:MET:CA   | 2.24                     | 0.84              |
| 1:F:287:ILE:HG12 | 1:H:65:LEU:HG   | 1.58                     | 0.84              |
| 1:B:74:GLY:O     | 1:B:75:ILE:CG1  | 2.24                     | 0.84              |
| 1:H:287:ILE:HG12 | 1:J:65:LEU:HG   | 1.58                     | 0.84              |
| 1:C:290:ARG:NE   | 1:E:64:ILE:CD1  | 2.43                     | 0.82              |
| 1:B:290:ARG:NE   | 1:D:64:ILE:CD1  | 2.43                     | 0.82              |
| 1:E:290:ARG:NE   | 1:G:64:ILE:CD1  | 2.43                     | 0.82              |
| 1:F:290:ARG:NE   | 1:H:64:ILE:CD1  | 2.43                     | 0.82              |
| 1:H:290:ARG:NE   | 1:J:64:ILE:CD1  | 2.43                     | 0.81              |
| 1:I:290:ARG:NE   | 1:K:64:ILE:CD1  | 2.43                     | 0.81              |
| 1:G:290:ARG:NE   | 1:I:64:ILE:CD1  | 2.43                     | 0.81              |
| 1:A:290:ARG:NE   | 1:C:64:ILE:CD1  | 2.43                     | 0.81              |
| 1:D:290:ARG:NE   | 1:F:64:ILE:CD1  | 2.43                     | 0.81              |
| 1:F:74:GLY:C     | 1:F:75:ILE:HG13 | 2.07                     | 0.80              |
| 1:H:74:GLY:C     | 1:H:75:ILE:HG13 | 2.07                     | 0.80              |
| 1:K:74:GLY:C     | 1:K:75:ILE:HG13 | 2.07                     | 0.80              |
| 1:I:74:GLY:C     | 1:I:75:ILE:HG13 | 2.07                     | 0.80              |
| 1:J:74:GLY:C     | 1:J:75:ILE:HG13 | 2.07                     | 0.80              |
| 1:D:74:GLY:C     | 1:D:75:ILE:HG13 | 2.07                     | 0.80              |
| 1:B:74:GLY:C     | 1:B:75:ILE:HG13 | 2.06                     | 0.80              |
| 1:G:74:GLY:C     | 1:G:75:ILE:HG13 | 2.07                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:287:ILE:HA  | 1:J:64:ILE:HD13 | 1.64                     | 0.80              |
| 1:F:287:ILE:HA  | 1:H:64:ILE:HD13 | 1.64                     | 0.80              |
| 1:B:287:ILE:HA  | 1:D:64:ILE:HD13 | 1.64                     | 0.79              |
| 1:E:74:GLY:C    | 1:E:75:ILE:HG13 | 2.07                     | 0.79              |
| 1:D:287:ILE:HA  | 1:F:64:ILE:HD13 | 1.65                     | 0.79              |
| 1:I:287:ILE:HA  | 1:K:64:ILE:CD1  | 2.12                     | 0.79              |
| 1:G:287:ILE:HA  | 1:I:64:ILE:CD1  | 2.12                     | 0.79              |
| 1:C:74:GLY:C    | 1:C:75:ILE:HG13 | 2.07                     | 0.79              |
| 1:A:74:GLY:C    | 1:A:75:ILE:HG13 | 2.06                     | 0.79              |
| 1:B:287:ILE:HA  | 1:D:64:ILE:CD1  | 2.12                     | 0.79              |
| 1:D:287:ILE:HA  | 1:F:64:ILE:CD1  | 2.12                     | 0.79              |
| 1:E:287:ILE:HA  | 1:G:64:ILE:CD1  | 2.12                     | 0.79              |
| 1:I:287:ILE:HA  | 1:K:64:ILE:HD13 | 1.64                     | 0.79              |
| 1:F:287:ILE:HA  | 1:H:64:ILE:CD1  | 2.12                     | 0.79              |
| 1:G:287:ILE:HA  | 1:I:64:ILE:HD13 | 1.64                     | 0.78              |
| 1:H:287:ILE:HA  | 1:J:64:ILE:CD1  | 2.12                     | 0.78              |
| 1:A:287:ILE:HA  | 1:C:64:ILE:CD1  | 2.12                     | 0.78              |
| 1:A:287:ILE:HA  | 1:C:64:ILE:HD13 | 1.64                     | 0.78              |
| 1:C:35:VAL:HG21 | 1:C:81:ASP:HB3  | 1.66                     | 0.78              |
| 1:C:287:ILE:HA  | 1:E:64:ILE:CD1  | 2.12                     | 0.78              |
| 1:C:287:ILE:HA  | 1:E:64:ILE:HD13 | 1.64                     | 0.78              |
| 1:E:287:ILE:HA  | 1:G:64:ILE:HD13 | 1.65                     | 0.78              |
| 1:E:35:VAL:HG21 | 1:E:81:ASP:HB3  | 1.66                     | 0.78              |
| 1:I:35:VAL:HG21 | 1:I:81:ASP:HB3  | 1.66                     | 0.78              |
| 1:K:35:VAL:HG21 | 1:K:81:ASP:HB3  | 1.66                     | 0.77              |
| 1:E:290:ARG:NE  | 1:G:64:ILE:HD13 | 2.00                     | 0.77              |
| 1:G:35:VAL:HG21 | 1:G:81:ASP:HB3  | 1.66                     | 0.77              |
| 1:G:290:ARG:NE  | 1:I:64:ILE:HD13 | 2.00                     | 0.77              |
| 1:A:35:VAL:HG21 | 1:A:81:ASP:HB3  | 1.66                     | 0.77              |
| 1:D:35:VAL:HG21 | 1:D:81:ASP:HB3  | 1.66                     | 0.77              |
| 1:B:35:VAL:HG21 | 1:B:81:ASP:HB3  | 1.66                     | 0.77              |
| 1:E:290:ARG:CZ  | 1:G:64:ILE:CG1  | 2.63                     | 0.77              |
| 1:J:35:VAL:HG21 | 1:J:81:ASP:HB3  | 1.66                     | 0.77              |
| 1:A:290:ARG:CZ  | 1:C:64:ILE:CG1  | 2.63                     | 0.76              |
| 1:C:290:ARG:CZ  | 1:E:64:ILE:CG1  | 2.63                     | 0.76              |
| 1:I:290:ARG:NH1 | 1:K:64:ILE:CG1  | 2.48                     | 0.76              |
| 1:I:290:ARG:NE  | 1:K:64:ILE:HD13 | 2.00                     | 0.76              |
| 1:I:290:ARG:CZ  | 1:K:64:ILE:CG1  | 2.63                     | 0.76              |
| 1:A:290:ARG:NE  | 1:C:64:ILE:HD13 | 2.00                     | 0.76              |
| 1:B:288:ASP:OD1 | 1:D:53:TYR:CZ   | 2.39                     | 0.76              |
| 1:C:290:ARG:NE  | 1:E:64:ILE:HD13 | 2.00                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:35:VAL:HG21 | 1:F:81:ASP:HB3  | 1.66                     | 0.76              |
| 1:G:290:ARG:NH1 | 1:I:64:ILE:CG1  | 2.48                     | 0.76              |
| 1:G:288:ASP:OD1 | 1:I:53:TYR:CZ   | 2.39                     | 0.76              |
| 1:H:35:VAL:HG21 | 1:H:81:ASP:HB3  | 1.66                     | 0.76              |
| 1:H:290:ARG:CZ  | 1:J:64:ILE:CG1  | 2.63                     | 0.76              |
| 1:C:288:ASP:OD1 | 1:E:53:TYR:CZ   | 2.39                     | 0.76              |
| 1:D:140:LEU:O   | 1:D:342:GLY:HA3 | 1.86                     | 0.76              |
| 1:D:288:ASP:OD1 | 1:F:53:TYR:CZ   | 2.39                     | 0.76              |
| 1:D:290:ARG:CZ  | 1:F:64:ILE:CG1  | 2.63                     | 0.76              |
| 1:E:288:ASP:OD1 | 1:G:53:TYR:CZ   | 2.39                     | 0.76              |
| 1:I:288:ASP:OD1 | 1:K:53:TYR:CZ   | 2.39                     | 0.76              |
| 1:A:290:ARG:NH1 | 1:C:64:ILE:CG1  | 2.48                     | 0.76              |
| 1:E:290:ARG:NH1 | 1:G:64:ILE:CG1  | 2.48                     | 0.76              |
| 1:H:290:ARG:NE  | 1:J:64:ILE:HD13 | 2.00                     | 0.76              |
| 1:A:288:ASP:OD1 | 1:C:53:TYR:CZ   | 2.39                     | 0.76              |
| 1:C:290:ARG:NH1 | 1:E:64:ILE:CG1  | 2.48                     | 0.76              |
| 1:F:290:ARG:CZ  | 1:H:64:ILE:CG1  | 2.63                     | 0.75              |
| 1:G:290:ARG:CZ  | 1:I:64:ILE:CG1  | 2.63                     | 0.75              |
| 1:F:288:ASP:OD1 | 1:H:53:TYR:CZ   | 2.39                     | 0.75              |
| 1:F:290:ARG:NE  | 1:H:64:ILE:HD13 | 2.00                     | 0.75              |
| 1:H:140:LEU:O   | 1:H:342:GLY:HA3 | 1.86                     | 0.75              |
| 1:B:290:ARG:CZ  | 1:D:64:ILE:CG1  | 2.63                     | 0.75              |
| 1:F:140:LEU:O   | 1:F:342:GLY:HA3 | 1.86                     | 0.75              |
| 1:J:72:GLU:O    | 1:J:73:HIS:CB   | 2.34                     | 0.75              |
| 1:A:72:GLU:O    | 1:A:73:HIS:CB   | 2.34                     | 0.75              |
| 1:D:72:GLU:O    | 1:D:73:HIS:CB   | 2.34                     | 0.75              |
| 1:D:290:ARG:NE  | 1:F:64:ILE:HD13 | 2.00                     | 0.75              |
| 1:I:72:GLU:O    | 1:I:73:HIS:CB   | 2.34                     | 0.75              |
| 1:K:140:LEU:O   | 1:K:342:GLY:HA3 | 1.86                     | 0.75              |
| 1:B:290:ARG:NH1 | 1:D:64:ILE:CG1  | 2.48                     | 0.75              |
| 1:C:140:LEU:O   | 1:C:342:GLY:HA3 | 1.86                     | 0.75              |
| 1:E:72:GLU:O    | 1:E:73:HIS:CB   | 2.34                     | 0.75              |
| 1:E:140:LEU:O   | 1:E:342:GLY:HA3 | 1.86                     | 0.75              |
| 1:H:288:ASP:OD1 | 1:J:53:TYR:CZ   | 2.39                     | 0.75              |
| 1:B:290:ARG:NE  | 1:D:64:ILE:HD13 | 2.00                     | 0.75              |
| 1:B:140:LEU:O   | 1:B:342:GLY:HA3 | 1.86                     | 0.74              |
| 1:J:140:LEU:O   | 1:J:342:GLY:HA3 | 1.86                     | 0.74              |
| 1:A:140:LEU:O   | 1:A:342:GLY:HA3 | 1.86                     | 0.74              |
| 1:K:72:GLU:O    | 1:K:73:HIS:CB   | 2.34                     | 0.74              |
| 1:C:72:GLU:O    | 1:C:73:HIS:CB   | 2.34                     | 0.74              |
| 1:G:140:LEU:O   | 1:G:342:GLY:HA3 | 1.86                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:290:ARG:NH1  | 1:F:64:ILE:CG1   | 2.48                     | 0.74              |
| 1:G:171:LEU:HD22 | 1:I:45:VAL:HG11  | 1.69                     | 0.74              |
| 1:A:286:ASP:HB2  | 1:C:46:GLY:C     | 2.13                     | 0.74              |
| 1:H:72:GLU:O     | 1:H:73:HIS:CB    | 2.34                     | 0.74              |
| 1:I:286:ASP:HB2  | 1:K:46:GLY:C     | 2.13                     | 0.74              |
| 1:I:140:LEU:O    | 1:I:342:GLY:HA3  | 1.86                     | 0.74              |
| 1:F:72:GLU:O     | 1:F:73:HIS:CB    | 2.34                     | 0.73              |
| 1:G:72:GLU:O     | 1:G:73:HIS:CB    | 2.34                     | 0.73              |
| 1:G:286:ASP:HB2  | 1:I:46:GLY:C     | 2.13                     | 0.73              |
| 1:I:287:ILE:HG21 | 1:K:65:LEU:HD11  | 1.69                     | 0.73              |
| 1:B:286:ASP:HB2  | 1:D:46:GLY:C     | 2.13                     | 0.73              |
| 1:C:286:ASP:HB2  | 1:E:46:GLY:C     | 2.13                     | 0.73              |
| 1:D:286:ASP:HB2  | 1:F:46:GLY:C     | 2.13                     | 0.73              |
| 1:F:290:ARG:NH1  | 1:H:64:ILE:CG1   | 2.48                     | 0.73              |
| 1:H:286:ASP:HB2  | 1:J:46:GLY:C     | 2.13                     | 0.73              |
| 1:F:286:ASP:HB2  | 1:H:46:GLY:C     | 2.13                     | 0.73              |
| 1:I:171:LEU:HD22 | 1:K:45:VAL:HG11  | 1.69                     | 0.73              |
| 1:E:286:ASP:HB2  | 1:G:46:GLY:C     | 2.13                     | 0.73              |
| 1:G:287:ILE:HG21 | 1:I:65:LEU:HD11  | 1.69                     | 0.73              |
| 1:E:287:ILE:HG21 | 1:G:65:LEU:HD11  | 1.69                     | 0.73              |
| 1:B:72:GLU:O     | 1:B:73:HIS:CB    | 2.34                     | 0.73              |
| 1:B:287:ILE:HG21 | 1:D:65:LEU:HD11  | 1.69                     | 0.73              |
| 1:D:287:ILE:HG21 | 1:F:65:LEU:HD11  | 1.69                     | 0.73              |
| 1:C:287:ILE:HG21 | 1:E:65:LEU:HD11  | 1.69                     | 0.72              |
| 1:A:287:ILE:HG21 | 1:C:65:LEU:HD11  | 1.69                     | 0.72              |
| 1:H:290:ARG:NH1  | 1:J:64:ILE:CG1   | 2.48                     | 0.72              |
| 1:B:171:LEU:HD22 | 1:D:45:VAL:HG11  | 1.69                     | 0.72              |
| 1:F:287:ILE:HG21 | 1:H:65:LEU:HD11  | 1.69                     | 0.72              |
| 1:B:212:ILE:HD11 | 1:B:248:ILE:HG13 | 1.72                     | 0.72              |
| 1:D:212:ILE:HD11 | 1:D:248:ILE:HG13 | 1.72                     | 0.72              |
| 1:C:142:LEU:HG   | 1:C:147:ARG:O    | 1.90                     | 0.72              |
| 1:E:212:ILE:HD11 | 1:E:248:ILE:HG13 | 1.72                     | 0.72              |
| 1:G:212:ILE:HD11 | 1:G:248:ILE:HG13 | 1.72                     | 0.72              |
| 1:C:212:ILE:HD11 | 1:C:248:ILE:HG13 | 1.72                     | 0.72              |
| 1:H:142:LEU:HG   | 1:H:147:ARG:O    | 1.90                     | 0.72              |
| 1:H:287:ILE:HG21 | 1:J:65:LEU:HD11  | 1.69                     | 0.72              |
| 1:I:142:LEU:HG   | 1:I:147:ARG:O    | 1.90                     | 0.72              |
| 1:I:212:ILE:HD11 | 1:I:248:ILE:HG13 | 1.72                     | 0.72              |
| 1:B:142:LEU:HG   | 1:B:147:ARG:O    | 1.90                     | 0.72              |
| 1:C:213:LYS:HA   | 1:C:217:CYS:SG   | 2.30                     | 0.72              |
| 1:E:142:LEU:HG   | 1:E:147:ARG:O    | 1.90                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:142:LEU:HG   | 1:A:147:ARG:O    | 1.90                     | 0.71              |
| 1:B:213:LYS:HA   | 1:B:217:CYS:SG   | 2.30                     | 0.71              |
| 1:D:142:LEU:HG   | 1:D:147:ARG:O    | 1.90                     | 0.71              |
| 1:K:212:ILE:HD11 | 1:K:248:ILE:HG13 | 1.72                     | 0.71              |
| 1:E:213:LYS:HA   | 1:E:217:CYS:SG   | 2.30                     | 0.71              |
| 1:G:290:ARG:CZ   | 1:I:64:ILE:CD1   | 2.69                     | 0.71              |
| 1:F:212:ILE:HD11 | 1:F:248:ILE:HG13 | 1.72                     | 0.71              |
| 1:H:290:ARG:CZ   | 1:J:64:ILE:CD1   | 2.69                     | 0.71              |
| 1:J:142:LEU:HG   | 1:J:147:ARG:O    | 1.90                     | 0.71              |
| 1:A:171:LEU:CD2  | 1:C:45:VAL:CG1   | 2.46                     | 0.71              |
| 1:A:212:ILE:HD11 | 1:A:248:ILE:HG13 | 1.72                     | 0.71              |
| 1:A:290:ARG:CZ   | 1:C:64:ILE:CD1   | 2.68                     | 0.71              |
| 1:I:290:ARG:CZ   | 1:K:64:ILE:CD1   | 2.69                     | 0.71              |
| 1:K:142:LEU:HG   | 1:K:147:ARG:O    | 1.90                     | 0.71              |
| 1:D:171:LEU:HD22 | 1:F:45:VAL:HG11  | 1.69                     | 0.71              |
| 1:D:213:LYS:HA   | 1:D:217:CYS:SG   | 2.30                     | 0.71              |
| 1:D:290:ARG:CZ   | 1:F:64:ILE:CD1   | 2.68                     | 0.71              |
| 1:C:290:ARG:CZ   | 1:E:64:ILE:CD1   | 2.68                     | 0.71              |
| 1:K:213:LYS:HA   | 1:K:217:CYS:SG   | 2.30                     | 0.71              |
| 1:A:213:LYS:HA   | 1:A:217:CYS:SG   | 2.30                     | 0.71              |
| 1:D:155:SER:O    | 1:D:301:GLY:HA3  | 1.91                     | 0.71              |
| 1:F:142:LEU:HG   | 1:F:147:ARG:O    | 1.90                     | 0.71              |
| 1:F:213:LYS:HA   | 1:F:217:CYS:SG   | 2.30                     | 0.71              |
| 1:G:213:LYS:HA   | 1:G:217:CYS:SG   | 2.30                     | 0.71              |
| 1:K:155:SER:O    | 1:K:301:GLY:HA3  | 1.91                     | 0.71              |
| 1:D:171:LEU:CD2  | 1:F:45:VAL:CG1   | 2.46                     | 0.70              |
| 1:G:142:LEU:HG   | 1:G:147:ARG:O    | 1.90                     | 0.70              |
| 1:H:155:SER:O    | 1:H:301:GLY:HA3  | 1.91                     | 0.70              |
| 1:E:290:ARG:CZ   | 1:G:64:ILE:CD1   | 2.68                     | 0.70              |
| 1:F:290:ARG:CZ   | 1:H:64:ILE:CD1   | 2.69                     | 0.70              |
| 1:I:213:LYS:HA   | 1:I:217:CYS:SG   | 2.30                     | 0.70              |
| 1:J:213:LYS:HA   | 1:J:217:CYS:SG   | 2.30                     | 0.70              |
| 1:B:155:SER:O    | 1:B:301:GLY:HA3  | 1.91                     | 0.70              |
| 1:B:290:ARG:CZ   | 1:D:64:ILE:CD1   | 2.69                     | 0.70              |
| 1:J:212:ILE:HD11 | 1:J:248:ILE:HG13 | 1.72                     | 0.70              |
| 1:I:155:SER:O    | 1:I:301:GLY:HA3  | 1.91                     | 0.70              |
| 1:H:212:ILE:HD11 | 1:H:248:ILE:HG13 | 1.72                     | 0.70              |
| 1:G:287:ILE:HG21 | 1:I:65:LEU:CG    | 2.22                     | 0.70              |
| 1:H:213:LYS:HA   | 1:H:217:CYS:SG   | 2.31                     | 0.70              |
| 1:A:155:SER:O    | 1:A:301:GLY:HA3  | 1.91                     | 0.70              |
| 1:F:287:ILE:HG21 | 1:H:65:LEU:CG    | 2.22                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:155:SER:O    | 1:F:301:GLY:HA3  | 1.91                     | 0.69              |
| 1:F:171:LEU:HD22 | 1:H:45:VAL:HG11  | 1.69                     | 0.69              |
| 1:G:155:SER:O    | 1:G:301:GLY:HA3  | 1.91                     | 0.69              |
| 1:D:287:ILE:HG21 | 1:F:65:LEU:CG    | 2.22                     | 0.69              |
| 1:E:287:ILE:HG21 | 1:G:65:LEU:CG    | 2.22                     | 0.69              |
| 1:I:287:ILE:HG21 | 1:K:65:LEU:CG    | 2.22                     | 0.69              |
| 1:A:33:SER:OG    | 1:A:85:ILE:HD13  | 1.92                     | 0.69              |
| 1:E:155:SER:O    | 1:E:301:GLY:HA3  | 1.91                     | 0.69              |
| 1:I:33:SER:OG    | 1:I:85:ILE:HD13  | 1.92                     | 0.69              |
| 1:J:155:SER:O    | 1:J:301:GLY:HA3  | 1.91                     | 0.69              |
| 1:G:173:HIS:HE1  | 1:I:45:VAL:CG1   | 2.03                     | 0.69              |
| 1:A:171:LEU:HD22 | 1:C:45:VAL:HG11  | 1.69                     | 0.69              |
| 1:C:33:SER:OG    | 1:C:85:ILE:HD13  | 1.92                     | 0.69              |
| 1:C:155:SER:O    | 1:C:301:GLY:HA3  | 1.91                     | 0.69              |
| 1:K:33:SER:OG    | 1:K:85:ILE:HD13  | 1.92                     | 0.69              |
| 1:A:173:HIS:HE1  | 1:C:45:VAL:CG1   | 2.03                     | 0.69              |
| 1:H:287:ILE:HG21 | 1:J:65:LEU:CG    | 2.22                     | 0.69              |
| 1:C:173:HIS:HE1  | 1:E:45:VAL:CG1   | 2.03                     | 0.69              |
| 1:G:33:SER:OG    | 1:G:85:ILE:HD13  | 1.92                     | 0.69              |
| 1:E:33:SER:OG    | 1:E:85:ILE:HD13  | 1.92                     | 0.69              |
| 1:J:33:SER:OG    | 1:J:85:ILE:HD13  | 1.92                     | 0.69              |
| 1:B:33:SER:OG    | 1:B:85:ILE:HD13  | 1.92                     | 0.68              |
| 1:C:287:ILE:HG21 | 1:E:65:LEU:CG    | 2.22                     | 0.68              |
| 1:C:171:LEU:HD22 | 1:E:45:VAL:HG11  | 1.69                     | 0.68              |
| 1:D:33:SER:OG    | 1:D:85:ILE:HD13  | 1.92                     | 0.68              |
| 1:F:33:SER:OG    | 1:F:85:ILE:HD13  | 1.92                     | 0.68              |
| 1:A:287:ILE:HG21 | 1:C:65:LEU:CG    | 2.22                     | 0.68              |
| 1:B:287:ILE:HG21 | 1:D:65:LEU:CG    | 2.22                     | 0.68              |
| 1:H:171:LEU:HD22 | 1:J:45:VAL:HG11  | 1.70                     | 0.68              |
| 1:H:33:SER:OG    | 1:H:85:ILE:HD13  | 1.92                     | 0.68              |
| 1:G:116:ARG:HD3  | 1:G:370:VAL:HG11 | 1.75                     | 0.68              |
| 1:K:32:PRO:HD2   | 1:K:59:GLN:OE1   | 1.94                     | 0.68              |
| 1:K:116:ARG:HD3  | 1:K:370:VAL:HG11 | 1.76                     | 0.68              |
| 1:C:171:LEU:CD2  | 1:E:45:VAL:CG1   | 2.46                     | 0.67              |
| 1:J:32:PRO:HD2   | 1:J:59:GLN:OE1   | 1.94                     | 0.67              |
| 1:A:32:PRO:HD2   | 1:A:59:GLN:OE1   | 1.94                     | 0.67              |
| 1:E:32:PRO:HD2   | 1:E:59:GLN:OE1   | 1.94                     | 0.67              |
| 1:A:317:ILE:HG22 | 1:A:327:ILE:HG13 | 1.77                     | 0.67              |
| 1:F:116:ARG:HD3  | 1:F:370:VAL:HG11 | 1.76                     | 0.67              |
| 1:H:116:ARG:HD3  | 1:H:370:VAL:HG11 | 1.76                     | 0.67              |
| 1:B:32:PRO:HD2   | 1:B:59:GLN:OE1   | 1.94                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:317:ILE:HG22 | 1:J:327:ILE:HG13 | 1.77                     | 0.67              |
| 1:B:286:ASP:CG   | 1:D:47:MET:HA    | 2.19                     | 0.67              |
| 1:D:32:PRO:HD2   | 1:D:59:GLN:OE1   | 1.94                     | 0.67              |
| 1:C:287:ILE:HG21 | 1:E:65:LEU:HD21  | 1.77                     | 0.67              |
| 1:C:317:ILE:HG22 | 1:C:327:ILE:HG13 | 1.77                     | 0.67              |
| 1:E:287:ILE:HG21 | 1:G:65:LEU:HD21  | 1.77                     | 0.67              |
| 1:F:287:ILE:HG21 | 1:H:65:LEU:HD21  | 1.77                     | 0.67              |
| 1:F:317:ILE:HG22 | 1:F:327:ILE:HG13 | 1.77                     | 0.67              |
| 1:H:32:PRO:HD2   | 1:H:59:GLN:OE1   | 1.94                     | 0.67              |
| 1:G:317:ILE:HG22 | 1:G:327:ILE:HG13 | 1.77                     | 0.67              |
| 1:I:32:PRO:HD2   | 1:I:59:GLN:OE1   | 1.94                     | 0.67              |
| 1:C:116:ARG:HD3  | 1:C:370:VAL:HG11 | 1.76                     | 0.67              |
| 1:D:286:ASP:CG   | 1:F:47:MET:HA    | 2.19                     | 0.67              |
| 1:E:171:LEU:HD22 | 1:G:45:VAL:HG11  | 1.70                     | 0.67              |
| 1:I:116:ARG:HD3  | 1:I:370:VAL:HG11 | 1.76                     | 0.67              |
| 1:D:287:ILE:HG21 | 1:F:65:LEU:HD21  | 1.77                     | 0.67              |
| 1:E:317:ILE:HG22 | 1:E:327:ILE:HG13 | 1.77                     | 0.67              |
| 1:H:173:HIS:HE1  | 1:J:45:VAL:CG1   | 2.03                     | 0.67              |
| 1:H:286:ASP:CG   | 1:J:47:MET:HA    | 2.19                     | 0.67              |
| 1:H:287:ILE:HG21 | 1:J:65:LEU:HD21  | 1.77                     | 0.67              |
| 1:I:286:ASP:OD1  | 1:K:46:GLY:O     | 2.13                     | 0.67              |
| 1:A:287:ILE:HG21 | 1:C:65:LEU:HD21  | 1.77                     | 0.67              |
| 1:C:286:ASP:CG   | 1:E:47:MET:HA    | 2.19                     | 0.67              |
| 1:D:116:ARG:HD3  | 1:D:370:VAL:HG11 | 1.76                     | 0.67              |
| 1:G:32:PRO:HD2   | 1:G:59:GLN:OE1   | 1.94                     | 0.67              |
| 1:G:286:ASP:OD1  | 1:I:46:GLY:O     | 2.13                     | 0.67              |
| 1:H:317:ILE:HG22 | 1:H:327:ILE:HG13 | 1.77                     | 0.67              |
| 1:B:173:HIS:HE1  | 1:D:45:VAL:CG1   | 2.03                     | 0.66              |
| 1:D:317:ILE:HG22 | 1:D:327:ILE:HG13 | 1.77                     | 0.66              |
| 1:I:173:HIS:HE1  | 1:K:45:VAL:CG1   | 2.03                     | 0.66              |
| 1:I:286:ASP:CG   | 1:K:47:MET:HA    | 2.19                     | 0.66              |
| 1:E:116:ARG:HD3  | 1:E:370:VAL:HG11 | 1.76                     | 0.66              |
| 1:E:286:ASP:CG   | 1:G:47:MET:HA    | 2.19                     | 0.66              |
| 1:G:286:ASP:CG   | 1:I:47:MET:HA    | 2.19                     | 0.66              |
| 1:G:287:ILE:HG21 | 1:I:65:LEU:HD21  | 1.77                     | 0.66              |
| 1:A:286:ASP:CG   | 1:C:47:MET:HA    | 2.19                     | 0.66              |
| 1:I:317:ILE:HG22 | 1:I:327:ILE:HG13 | 1.77                     | 0.66              |
| 1:B:287:ILE:HG21 | 1:D:65:LEU:HD21  | 1.77                     | 0.66              |
| 1:C:32:PRO:HD2   | 1:C:59:GLN:OE1   | 1.94                     | 0.66              |
| 1:E:173:HIS:HE1  | 1:G:45:VAL:CG1   | 2.03                     | 0.66              |
| 1:F:32:PRO:HD2   | 1:F:59:GLN:OE1   | 1.94                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:116:ARG:HD3  | 1:J:370:VAL:HG11 | 1.76                     | 0.66              |
| 1:B:116:ARG:HD3  | 1:B:370:VAL:HG11 | 1.75                     | 0.66              |
| 1:D:173:HIS:HE1  | 1:F:45:VAL:CG1   | 2.03                     | 0.66              |
| 1:F:286:ASP:CG   | 1:H:47:MET:HA    | 2.19                     | 0.66              |
| 1:K:317:ILE:HG22 | 1:K:327:ILE:HG13 | 1.77                     | 0.66              |
| 1:I:242:LEU:HD12 | 1:I:243:PRO:HD2  | 1.78                     | 0.66              |
| 1:B:317:ILE:HG22 | 1:B:327:ILE:HG13 | 1.77                     | 0.66              |
| 1:E:286:ASP:OD1  | 1:G:46:GLY:O     | 2.13                     | 0.66              |
| 1:F:242:LEU:HD12 | 1:F:243:PRO:HD2  | 1.78                     | 0.66              |
| 1:F:286:ASP:OD1  | 1:H:46:GLY:O     | 2.13                     | 0.66              |
| 1:I:287:ILE:HG21 | 1:K:65:LEU:HD21  | 1.77                     | 0.66              |
| 1:A:116:ARG:HD3  | 1:A:370:VAL:HG11 | 1.76                     | 0.66              |
| 1:G:242:LEU:HD12 | 1:G:243:PRO:HD2  | 1.78                     | 0.66              |
| 1:H:242:LEU:HD12 | 1:H:243:PRO:HD2  | 1.78                     | 0.66              |
| 1:H:286:ASP:OD1  | 1:J:46:GLY:O     | 2.13                     | 0.66              |
| 1:K:242:LEU:HD12 | 1:K:243:PRO:HD2  | 1.78                     | 0.66              |
| 1:B:286:ASP:OD1  | 1:D:46:GLY:O     | 2.13                     | 0.66              |
| 1:D:286:ASP:OD1  | 1:F:46:GLY:O     | 2.13                     | 0.66              |
| 1:D:155:SER:OG   | 1:D:303:THR:HB   | 1.97                     | 0.65              |
| 1:J:242:LEU:HD12 | 1:J:243:PRO:HD2  | 1.78                     | 0.65              |
| 1:C:155:SER:OG   | 1:C:303:THR:HB   | 1.97                     | 0.65              |
| 1:D:39:ARG:HD2   | 1:D:66:THR:OG1   | 1.97                     | 0.65              |
| 1:B:242:LEU:HD12 | 1:B:243:PRO:HD2  | 1.78                     | 0.65              |
| 1:D:242:LEU:HD12 | 1:D:243:PRO:HD2  | 1.78                     | 0.65              |
| 1:G:155:SER:OG   | 1:G:303:THR:HB   | 1.97                     | 0.65              |
| 1:I:155:SER:OG   | 1:I:303:THR:HB   | 1.97                     | 0.65              |
| 1:D:74:GLY:H     | 1:D:108:ALA:CB   | 2.10                     | 0.65              |
| 1:E:242:LEU:HD12 | 1:E:243:PRO:HD2  | 1.78                     | 0.65              |
| 1:K:74:GLY:H     | 1:K:108:ALA:CB   | 2.10                     | 0.65              |
| 1:A:287:ILE:HB   | 1:C:64:ILE:CG2   | 2.27                     | 0.65              |
| 1:B:39:ARG:HD2   | 1:B:66:THR:OG1   | 1.97                     | 0.65              |
| 1:B:74:GLY:H     | 1:B:108:ALA:CB   | 2.10                     | 0.65              |
| 1:C:286:ASP:OD1  | 1:E:46:GLY:O     | 2.13                     | 0.65              |
| 1:F:39:ARG:HD2   | 1:F:66:THR:OG1   | 1.97                     | 0.65              |
| 1:F:74:GLY:H     | 1:F:108:ALA:CB   | 2.10                     | 0.65              |
| 1:K:39:ARG:HD2   | 1:K:66:THR:OG1   | 1.97                     | 0.65              |
| 1:C:335:ARG:HA   | 1:C:338:SER:OG   | 1.97                     | 0.65              |
| 1:G:39:ARG:HD2   | 1:G:66:THR:OG1   | 1.97                     | 0.65              |
| 1:I:39:ARG:HD2   | 1:I:66:THR:OG1   | 1.97                     | 0.65              |
| 1:A:155:SER:OG   | 1:A:303:THR:HB   | 1.97                     | 0.65              |
| 1:C:287:ILE:HB   | 1:E:64:ILE:CG2   | 2.27                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:335:ARG:HA   | 1:D:338:SER:OG  | 1.97                     | 0.65              |
| 1:E:335:ARG:HA   | 1:E:338:SER:OG  | 1.97                     | 0.65              |
| 1:F:335:ARG:HA   | 1:F:338:SER:OG  | 1.97                     | 0.65              |
| 1:A:335:ARG:HA   | 1:A:338:SER:OG  | 1.97                     | 0.65              |
| 1:G:192:ILE:HD12 | 1:G:253:GLU:HA  | 1.79                     | 0.65              |
| 1:H:155:SER:OG   | 1:H:303:THR:HB  | 1.96                     | 0.65              |
| 1:B:192:ILE:HD12 | 1:B:253:GLU:HA  | 1.79                     | 0.65              |
| 1:C:74:GLY:H     | 1:C:108:ALA:CB  | 2.10                     | 0.65              |
| 1:E:39:ARG:HD2   | 1:E:66:THR:OG1  | 1.97                     | 0.65              |
| 1:E:74:GLY:H     | 1:E:108:ALA:CB  | 2.10                     | 0.65              |
| 1:F:192:ILE:HD12 | 1:F:253:GLU:HA  | 1.79                     | 0.65              |
| 1:H:287:ILE:HB   | 1:J:64:ILE:CG2  | 2.27                     | 0.65              |
| 1:J:39:ARG:HD2   | 1:J:66:THR:OG1  | 1.97                     | 0.65              |
| 1:J:335:ARG:HA   | 1:J:338:SER:OG  | 1.97                     | 0.65              |
| 1:A:39:ARG:HD2   | 1:A:66:THR:OG1  | 1.97                     | 0.65              |
| 1:A:242:LEU:HD12 | 1:A:243:PRO:HD2 | 1.78                     | 0.65              |
| 1:D:192:ILE:HD12 | 1:D:253:GLU:HA  | 1.79                     | 0.65              |
| 1:I:74:GLY:H     | 1:I:108:ALA:CB  | 2.10                     | 0.65              |
| 1:I:192:ILE:HD12 | 1:I:253:GLU:HA  | 1.79                     | 0.65              |
| 1:K:192:ILE:HD12 | 1:K:253:GLU:HA  | 1.79                     | 0.65              |
| 1:A:286:ASP:OD1  | 1:C:46:GLY:O    | 2.13                     | 0.64              |
| 1:B:155:SER:OG   | 1:B:303:THR:HB  | 1.96                     | 0.64              |
| 1:E:287:ILE:HB   | 1:G:64:ILE:CG2  | 2.27                     | 0.64              |
| 1:F:287:ILE:HB   | 1:H:64:ILE:CG2  | 2.27                     | 0.64              |
| 1:G:35:VAL:HG21  | 1:G:81:ASP:CB   | 2.27                     | 0.64              |
| 1:G:335:ARG:HA   | 1:G:338:SER:OG  | 1.97                     | 0.64              |
| 1:J:155:SER:OG   | 1:J:303:THR:HB  | 1.97                     | 0.64              |
| 1:B:287:ILE:HB   | 1:D:64:ILE:CG2  | 2.27                     | 0.64              |
| 1:F:173:HIS:HE1  | 1:H:45:VAL:CG1  | 2.03                     | 0.64              |
| 1:G:287:ILE:HB   | 1:I:64:ILE:CG2  | 2.27                     | 0.64              |
| 1:H:335:ARG:HA   | 1:H:338:SER:OG  | 1.97                     | 0.64              |
| 1:I:35:VAL:HG21  | 1:I:81:ASP:CB   | 2.27                     | 0.64              |
| 1:B:335:ARG:HA   | 1:B:338:SER:OG  | 1.97                     | 0.64              |
| 1:D:287:ILE:HB   | 1:F:64:ILE:CG2  | 2.27                     | 0.64              |
| 1:H:39:ARG:HD2   | 1:H:66:THR:OG1  | 1.97                     | 0.64              |
| 1:H:74:GLY:H     | 1:H:108:ALA:CB  | 2.10                     | 0.64              |
| 1:H:192:ILE:HD12 | 1:H:253:GLU:HA  | 1.79                     | 0.64              |
| 1:J:74:GLY:H     | 1:J:108:ALA:CB  | 2.10                     | 0.64              |
| 1:C:35:VAL:HG21  | 1:C:81:ASP:CB   | 2.27                     | 0.64              |
| 1:F:155:SER:OG   | 1:F:303:THR:HB  | 1.96                     | 0.64              |
| 1:E:155:SER:OG   | 1:E:303:THR:HB  | 1.97                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:192:ILE:HD12 | 1:E:253:GLU:HA   | 1.79                     | 0.64              |
| 1:I:287:ILE:HB   | 1:K:64:ILE:CG2   | 2.27                     | 0.64              |
| 1:K:155:SER:OG   | 1:K:303:THR:HB   | 1.96                     | 0.64              |
| 1:D:35:VAL:HG21  | 1:D:81:ASP:CB    | 2.27                     | 0.64              |
| 1:C:39:ARG:HD2   | 1:C:66:THR:OG1   | 1.97                     | 0.64              |
| 1:C:242:LEU:HD12 | 1:C:243:PRO:HD2  | 1.78                     | 0.64              |
| 1:E:171:LEU:CD2  | 1:G:45:VAL:CG1   | 2.46                     | 0.64              |
| 1:I:335:ARG:HA   | 1:I:338:SER:OG   | 1.97                     | 0.64              |
| 1:A:74:GLY:H     | 1:A:108:ALA:CB   | 2.10                     | 0.64              |
| 1:B:35:VAL:HG21  | 1:B:81:ASP:CB    | 2.27                     | 0.64              |
| 1:B:287:ILE:HG13 | 1:D:61:LYS:HB3   | 1.80                     | 0.64              |
| 1:F:287:ILE:HG13 | 1:H:61:LYS:HB3   | 1.80                     | 0.64              |
| 1:J:192:ILE:HD12 | 1:J:253:GLU:HA   | 1.79                     | 0.64              |
| 1:A:192:ILE:HD12 | 1:A:253:GLU:HA   | 1.79                     | 0.64              |
| 1:A:35:VAL:HG21  | 1:A:81:ASP:CB    | 2.27                     | 0.63              |
| 1:E:287:ILE:HG21 | 1:G:65:LEU:CD1   | 2.28                     | 0.63              |
| 1:G:74:GLY:H     | 1:G:108:ALA:CB   | 2.10                     | 0.63              |
| 1:G:287:ILE:HG21 | 1:I:65:LEU:CD1   | 2.28                     | 0.63              |
| 1:C:192:ILE:HD12 | 1:C:253:GLU:HA   | 1.79                     | 0.63              |
| 1:H:35:VAL:HG21  | 1:H:81:ASP:CB    | 2.27                     | 0.63              |
| 1:I:287:ILE:HG21 | 1:K:65:LEU:CD1   | 2.28                     | 0.63              |
| 1:K:35:VAL:HG21  | 1:K:81:ASP:CB    | 2.27                     | 0.63              |
| 1:C:287:ILE:HG21 | 1:E:65:LEU:CD1   | 2.28                     | 0.63              |
| 1:K:335:ARG:HA   | 1:K:338:SER:OG   | 1.97                     | 0.63              |
| 1:E:35:VAL:HG21  | 1:E:81:ASP:CB    | 2.27                     | 0.63              |
| 1:D:287:ILE:HG21 | 1:F:65:LEU:CD1   | 2.28                     | 0.63              |
| 1:H:287:ILE:HG21 | 1:J:65:LEU:CD1   | 2.28                     | 0.63              |
| 1:A:287:ILE:HG21 | 1:C:65:LEU:CD1   | 2.28                     | 0.63              |
| 1:B:287:ILE:HG21 | 1:D:65:LEU:CD1   | 2.28                     | 0.63              |
| 1:G:287:ILE:HG13 | 1:I:61:LYS:HB3   | 1.80                     | 0.63              |
| 1:I:287:ILE:HG13 | 1:K:61:LYS:HB3   | 1.80                     | 0.63              |
| 1:J:248:ILE:H    | 1:J:248:ILE:HD13 | 1.64                     | 0.63              |
| 1:G:35:VAL:HG21  | 1:G:81:ASP:CG    | 2.24                     | 0.63              |
| 1:H:248:ILE:H    | 1:H:248:ILE:HD13 | 1.64                     | 0.63              |
| 1:H:287:ILE:HG13 | 1:J:61:LYS:HB3   | 1.80                     | 0.63              |
| 1:A:248:ILE:HD13 | 1:A:248:ILE:H    | 1.64                     | 0.62              |
| 1:B:248:ILE:H    | 1:B:248:ILE:HD13 | 1.64                     | 0.62              |
| 1:E:35:VAL:HG21  | 1:E:81:ASP:CG    | 2.24                     | 0.62              |
| 1:F:35:VAL:HG21  | 1:F:81:ASP:CB    | 2.27                     | 0.62              |
| 1:E:248:ILE:H    | 1:E:248:ILE:HD13 | 1.64                     | 0.62              |
| 1:G:248:ILE:HD13 | 1:G:248:ILE:H    | 1.64                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:248:ILE:HD13 | 1:F:248:ILE:H   | 1.64                     | 0.62              |
| 1:C:35:VAL:HG21  | 1:C:81:ASP:CG   | 2.24                     | 0.62              |
| 1:C:248:ILE:HD13 | 1:C:248:ILE:H   | 1.64                     | 0.62              |
| 1:I:35:VAL:HG21  | 1:I:81:ASP:CG   | 2.24                     | 0.62              |
| 1:A:287:ILE:HG13 | 1:C:61:LYS:HB3  | 1.80                     | 0.62              |
| 1:I:248:ILE:HD13 | 1:I:248:ILE:H   | 1.64                     | 0.62              |
| 1:B:35:VAL:HG21  | 1:B:81:ASP:CG   | 2.24                     | 0.62              |
| 1:F:287:ILE:HG21 | 1:H:65:LEU:CD1  | 2.28                     | 0.62              |
| 1:J:35:VAL:HG21  | 1:J:81:ASP:CB   | 2.27                     | 0.62              |
| 1:D:248:ILE:HD13 | 1:D:248:ILE:H   | 1.64                     | 0.62              |
| 1:D:287:ILE:HG13 | 1:F:61:LYS:HB3  | 1.80                     | 0.62              |
| 1:K:35:VAL:HG21  | 1:K:81:ASP:CG   | 2.24                     | 0.62              |
| 1:A:35:VAL:HG21  | 1:A:81:ASP:CG   | 2.24                     | 0.62              |
| 1:C:287:ILE:HG13 | 1:E:61:LYS:HB3  | 1.80                     | 0.62              |
| 1:J:35:VAL:HG21  | 1:J:81:ASP:CG   | 2.24                     | 0.62              |
| 1:H:35:VAL:HG21  | 1:H:81:ASP:CG   | 2.24                     | 0.61              |
| 1:J:170:ALA:H    | 1:J:375:PHE:HB3 | 1.65                     | 0.61              |
| 1:D:35:VAL:HG21  | 1:D:81:ASP:CG   | 2.24                     | 0.61              |
| 1:B:170:ALA:H    | 1:B:375:PHE:HB3 | 1.65                     | 0.61              |
| 1:I:287:ILE:HG12 | 1:K:61:LYS:O    | 2.01                     | 0.61              |
| 1:K:248:ILE:HD13 | 1:K:248:ILE:H   | 1.64                     | 0.61              |
| 1:B:287:ILE:HG12 | 1:D:61:LYS:O    | 2.01                     | 0.61              |
| 1:C:287:ILE:HG12 | 1:E:61:LYS:O    | 2.01                     | 0.61              |
| 1:D:170:ALA:H    | 1:D:375:PHE:HB3 | 1.65                     | 0.61              |
| 1:F:35:VAL:HG21  | 1:F:81:ASP:CG   | 2.24                     | 0.61              |
| 1:F:196:ARG:NH2  | 1:F:231:ALA:HA  | 2.16                     | 0.61              |
| 1:G:196:ARG:NH2  | 1:G:231:ALA:HA  | 2.16                     | 0.61              |
| 1:H:170:ALA:H    | 1:H:375:PHE:HB3 | 1.65                     | 0.61              |
| 1:K:196:ARG:NH2  | 1:K:231:ALA:HA  | 2.16                     | 0.61              |
| 1:E:287:ILE:HG13 | 1:G:61:LYS:HB3  | 1.80                     | 0.61              |
| 1:H:288:ASP:OD1  | 1:J:53:TYR:CE2  | 2.54                     | 0.61              |
| 1:A:288:ASP:OD1  | 1:C:53:TYR:CE2  | 2.54                     | 0.61              |
| 1:F:288:ASP:OD1  | 1:H:53:TYR:CE2  | 2.54                     | 0.61              |
| 1:H:196:ARG:NH2  | 1:H:231:ALA:HA  | 2.16                     | 0.61              |
| 1:A:196:ARG:NH2  | 1:A:231:ALA:HA  | 2.16                     | 0.61              |
| 1:C:288:ASP:OD1  | 1:E:53:TYR:CE2  | 2.54                     | 0.61              |
| 1:E:196:ARG:NH2  | 1:E:231:ALA:HA  | 2.16                     | 0.61              |
| 1:G:171:LEU:CD2  | 1:I:45:VAL:CG1  | 2.46                     | 0.61              |
| 1:I:288:ASP:OD1  | 1:K:53:TYR:CE2  | 2.54                     | 0.61              |
| 1:J:196:ARG:NH2  | 1:J:231:ALA:HA  | 2.16                     | 0.61              |
| 1:B:139:VAL:HA   | 1:B:165:ILE:CD1 | 2.31                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:287:ILE:HG12 | 1:G:61:LYS:O     | 2.01                     | 0.61              |
| 1:G:139:VAL:HA   | 1:G:165:ILE:CD1  | 2.31                     | 0.61              |
| 1:A:139:VAL:HA   | 1:A:165:ILE:CD1  | 2.31                     | 0.61              |
| 1:A:185:LEU:HD22 | 1:A:257:CYS:O    | 2.01                     | 0.61              |
| 1:B:196:ARG:NH2  | 1:B:231:ALA:HA   | 2.16                     | 0.61              |
| 1:B:288:ASP:OD1  | 1:D:53:TYR:CE2   | 2.54                     | 0.61              |
| 1:D:139:VAL:HA   | 1:D:165:ILE:CD1  | 2.31                     | 0.61              |
| 1:E:288:ASP:OD1  | 1:G:53:TYR:CE2   | 2.54                     | 0.61              |
| 1:G:287:ILE:HG12 | 1:I:61:LYS:O     | 2.01                     | 0.61              |
| 1:H:185:LEU:HD22 | 1:H:257:CYS:O    | 2.01                     | 0.61              |
| 1:H:287:ILE:HG12 | 1:J:61:LYS:O     | 2.01                     | 0.61              |
| 1:I:196:ARG:NH2  | 1:I:231:ALA:HA   | 2.16                     | 0.61              |
| 1:D:196:ARG:NH2  | 1:D:231:ALA:HA   | 2.16                     | 0.60              |
| 1:D:288:ASP:OD1  | 1:F:53:TYR:CE2   | 2.54                     | 0.60              |
| 1:G:288:ASP:OD1  | 1:I:53:TYR:CE2   | 2.54                     | 0.60              |
| 1:A:287:ILE:HG12 | 1:C:61:LYS:O     | 2.01                     | 0.60              |
| 1:D:287:ILE:HG12 | 1:F:61:LYS:O     | 2.01                     | 0.60              |
| 1:E:170:ALA:H    | 1:E:375:PHE:HB3  | 1.65                     | 0.60              |
| 1:F:139:VAL:HA   | 1:F:165:ILE:CD1  | 2.31                     | 0.60              |
| 1:K:139:VAL:HA   | 1:K:165:ILE:CD1  | 2.31                     | 0.60              |
| 1:F:170:ALA:H    | 1:F:375:PHE:HB3  | 1.65                     | 0.60              |
| 1:A:170:ALA:H    | 1:A:375:PHE:HB3  | 1.65                     | 0.60              |
| 1:C:139:VAL:HA   | 1:C:165:ILE:CD1  | 2.31                     | 0.60              |
| 1:C:170:ALA:H    | 1:C:375:PHE:HB3  | 1.65                     | 0.60              |
| 1:J:185:LEU:HD22 | 1:J:257:CYS:O    | 2.01                     | 0.60              |
| 1:F:185:LEU:HD22 | 1:F:257:CYS:O    | 2.01                     | 0.60              |
| 1:G:170:ALA:H    | 1:G:375:PHE:HB3  | 1.65                     | 0.60              |
| 1:H:139:VAL:HA   | 1:H:165:ILE:CD1  | 2.31                     | 0.60              |
| 1:I:170:ALA:H    | 1:I:375:PHE:HB3  | 1.65                     | 0.60              |
| 1:C:196:ARG:NH2  | 1:C:231:ALA:HA   | 2.16                     | 0.60              |
| 1:D:185:LEU:HD22 | 1:D:257:CYS:O    | 2.01                     | 0.60              |
| 1:E:139:VAL:HA   | 1:E:165:ILE:CD1  | 2.31                     | 0.60              |
| 1:I:139:VAL:HA   | 1:I:165:ILE:CD1  | 2.31                     | 0.60              |
| 1:F:287:ILE:HG12 | 1:H:61:LYS:O     | 2.01                     | 0.60              |
| 1:B:185:LEU:HD22 | 1:B:257:CYS:O    | 2.01                     | 0.60              |
| 1:F:171:LEU:CD2  | 1:H:45:VAL:CG1   | 2.46                     | 0.60              |
| 1:J:139:VAL:HA   | 1:J:165:ILE:CD1  | 2.31                     | 0.60              |
| 1:I:185:LEU:HD22 | 1:I:257:CYS:O    | 2.01                     | 0.60              |
| 1:K:170:ALA:H    | 1:K:375:PHE:HB3  | 1.65                     | 0.60              |
| 1:K:185:LEU:HD22 | 1:K:257:CYS:O    | 2.01                     | 0.60              |
| 1:K:260:THR:HG21 | 1:K:267:ILE:HG23 | 1.84                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:185:LEU:HD22 | 1:E:257:CYS:O    | 2.01                     | 0.59              |
| 1:H:260:THR:HG21 | 1:H:267:ILE:HG23 | 1.84                     | 0.59              |
| 1:I:260:THR:HG21 | 1:I:267:ILE:HG23 | 1.84                     | 0.59              |
| 1:B:260:THR:HG21 | 1:B:267:ILE:HG23 | 1.84                     | 0.59              |
| 1:G:185:LEU:HD22 | 1:G:257:CYS:O    | 2.01                     | 0.59              |
| 1:H:171:LEU:CD2  | 1:J:45:VAL:CG1   | 2.46                     | 0.59              |
| 1:C:185:LEU:HD22 | 1:C:257:CYS:O    | 2.01                     | 0.59              |
| 1:F:260:THR:HG21 | 1:F:267:ILE:HG23 | 1.84                     | 0.59              |
| 1:D:260:THR:HG21 | 1:D:267:ILE:HG23 | 1.85                     | 0.59              |
| 1:J:260:THR:HG21 | 1:J:267:ILE:HG23 | 1.84                     | 0.59              |
| 1:A:260:THR:HG21 | 1:A:267:ILE:HG23 | 1.85                     | 0.59              |
| 1:C:260:THR:HG21 | 1:C:267:ILE:HG23 | 1.85                     | 0.59              |
| 1:E:260:THR:HG21 | 1:E:267:ILE:HG23 | 1.84                     | 0.59              |
| 1:G:260:THR:HG21 | 1:G:267:ILE:HG23 | 1.85                     | 0.59              |
| 1:A:171:LEU:HD21 | 1:C:45:VAL:HG12  | 1.76                     | 0.58              |
| 1:I:171:LEU:CD2  | 1:K:45:VAL:CG1   | 2.46                     | 0.58              |
| 1:B:171:LEU:CD2  | 1:D:45:VAL:CG1   | 2.46                     | 0.58              |
| 1:B:287:ILE:HG21 | 1:D:65:LEU:CD2   | 2.34                     | 0.58              |
| 1:H:35:VAL:CG2   | 1:H:81:ASP:HB3   | 2.34                     | 0.58              |
| 1:A:35:VAL:CG2   | 1:A:81:ASP:HB3   | 2.34                     | 0.58              |
| 1:H:171:LEU:HD21 | 1:J:45:VAL:HG12  | 1.76                     | 0.58              |
| 1:G:312:ARG:HG3  | 1:G:312:ARG:HH11 | 1.69                     | 0.57              |
| 1:B:312:ARG:HH11 | 1:B:312:ARG:HG3  | 1.69                     | 0.57              |
| 1:C:287:ILE:HG21 | 1:E:65:LEU:CD2   | 2.34                     | 0.57              |
| 1:D:312:ARG:HG3  | 1:D:312:ARG:HH11 | 1.69                     | 0.57              |
| 1:G:180:LEU:HD23 | 1:G:261:LEU:HD23 | 1.87                     | 0.57              |
| 1:C:171:LEU:HD21 | 1:E:45:VAL:HG12  | 1.75                     | 0.57              |
| 1:H:180:LEU:HD23 | 1:H:261:LEU:HD23 | 1.87                     | 0.57              |
| 1:I:312:ARG:HH11 | 1:I:312:ARG:HG3  | 1.69                     | 0.57              |
| 1:A:180:LEU:HD23 | 1:A:261:LEU:HD23 | 1.87                     | 0.57              |
| 1:J:180:LEU:HD23 | 1:J:261:LEU:HD23 | 1.87                     | 0.57              |
| 1:J:312:ARG:HH11 | 1:J:312:ARG:HG3  | 1.70                     | 0.57              |
| 1:D:35:VAL:CG2   | 1:D:81:ASP:HB3   | 2.34                     | 0.57              |
| 1:D:287:ILE:HG21 | 1:F:65:LEU:CD2   | 2.34                     | 0.57              |
| 1:H:312:ARG:HH11 | 1:H:312:ARG:HG3  | 1.69                     | 0.57              |
| 1:I:180:LEU:HD23 | 1:I:261:LEU:HD23 | 1.87                     | 0.57              |
| 1:K:312:ARG:HH11 | 1:K:312:ARG:HG3  | 1.69                     | 0.57              |
| 1:A:312:ARG:HG3  | 1:A:312:ARG:HH11 | 1.69                     | 0.57              |
| 1:F:35:VAL:CG2   | 1:F:81:ASP:HB3   | 2.34                     | 0.57              |
| 1:F:180:LEU:HD23 | 1:F:261:LEU:HD23 | 1.87                     | 0.57              |
| 1:G:287:ILE:HG21 | 1:I:65:LEU:CD2   | 2.34                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:287:ILE:HG21 | 1:K:65:LEU:CD2   | 2.34                     | 0.57              |
| 1:B:35:VAL:CG2   | 1:B:81:ASP:HB3   | 2.34                     | 0.57              |
| 1:D:250:ILE:HG13 | 1:D:253:GLU:HB2  | 1.87                     | 0.57              |
| 1:F:171:LEU:HD21 | 1:H:45:VAL:HG12  | 1.76                     | 0.57              |
| 1:K:180:LEU:HD23 | 1:K:261:LEU:HD23 | 1.87                     | 0.57              |
| 1:A:139:VAL:HA   | 1:A:165:ILE:HD11 | 1.87                     | 0.57              |
| 1:B:139:VAL:HA   | 1:B:165:ILE:HD11 | 1.87                     | 0.57              |
| 1:B:250:ILE:HG13 | 1:B:253:GLU:HB2  | 1.87                     | 0.57              |
| 1:B:345:ILE:O    | 1:B:349:LEU:HG   | 2.05                     | 0.57              |
| 1:C:180:LEU:HD23 | 1:C:261:LEU:HD23 | 1.87                     | 0.57              |
| 1:E:180:LEU:HD23 | 1:E:261:LEU:HD23 | 1.87                     | 0.57              |
| 1:B:180:LEU:HD23 | 1:B:261:LEU:HD23 | 1.87                     | 0.57              |
| 1:E:287:ILE:HG21 | 1:G:65:LEU:CD2   | 2.34                     | 0.57              |
| 1:F:250:ILE:HG13 | 1:F:253:GLU:HB2  | 1.87                     | 0.57              |
| 1:J:139:VAL:HA   | 1:J:165:ILE:HD11 | 1.87                     | 0.57              |
| 1:A:287:ILE:HG21 | 1:C:65:LEU:CD2   | 2.34                     | 0.57              |
| 1:A:345:ILE:O    | 1:A:349:LEU:HG   | 2.05                     | 0.57              |
| 1:C:139:VAL:HA   | 1:C:165:ILE:HD11 | 1.87                     | 0.57              |
| 1:E:35:VAL:CG2   | 1:E:81:ASP:HB3   | 2.34                     | 0.57              |
| 1:E:312:ARG:HH11 | 1:E:312:ARG:HG3  | 1.69                     | 0.57              |
| 1:G:35:VAL:CG2   | 1:G:81:ASP:HB3   | 2.34                     | 0.57              |
| 1:G:139:VAL:HA   | 1:G:165:ILE:HD11 | 1.87                     | 0.57              |
| 1:I:139:VAL:HA   | 1:I:165:ILE:HD11 | 1.87                     | 0.57              |
| 1:J:35:VAL:CG2   | 1:J:81:ASP:HB3   | 2.34                     | 0.57              |
| 1:K:139:VAL:HA   | 1:K:165:ILE:HD11 | 1.87                     | 0.57              |
| 1:E:345:ILE:O    | 1:E:349:LEU:HG   | 2.05                     | 0.56              |
| 1:F:117:GLU:HA   | 1:F:367:PRO:CB   | 2.35                     | 0.56              |
| 1:H:139:VAL:HA   | 1:H:165:ILE:HD11 | 1.87                     | 0.56              |
| 1:I:242:LEU:CD1  | 1:I:243:PRO:HD2  | 2.35                     | 0.56              |
| 1:J:242:LEU:CD1  | 1:J:243:PRO:HD2  | 2.35                     | 0.56              |
| 1:K:250:ILE:HG13 | 1:K:253:GLU:HB2  | 1.87                     | 0.56              |
| 1:K:345:ILE:O    | 1:K:349:LEU:HG   | 2.05                     | 0.56              |
| 1:C:242:LEU:CD1  | 1:C:243:PRO:HD2  | 2.35                     | 0.56              |
| 1:D:180:LEU:HD23 | 1:D:261:LEU:HD23 | 1.87                     | 0.56              |
| 1:F:139:VAL:HA   | 1:F:165:ILE:HD11 | 1.87                     | 0.56              |
| 1:F:312:ARG:HH11 | 1:F:312:ARG:HG3  | 1.69                     | 0.56              |
| 1:G:166:TYR:CG   | 1:G:289:ILE:HG21 | 2.41                     | 0.56              |
| 1:A:117:GLU:HA   | 1:A:367:PRO:CB   | 2.35                     | 0.56              |
| 1:A:169:TYR:CD2  | 1:A:375:PHE:HA   | 2.40                     | 0.56              |
| 1:C:117:GLU:HA   | 1:C:367:PRO:CB   | 2.35                     | 0.56              |
| 1:C:312:ARG:HH11 | 1:C:312:ARG:HG3  | 1.69                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:139:VAL:HA   | 1:D:165:ILE:HD11 | 1.87                     | 0.56              |
| 1:E:166:TYR:CG   | 1:E:289:ILE:HG21 | 2.41                     | 0.56              |
| 1:E:171:LEU:HD21 | 1:G:45:VAL:HG12  | 1.76                     | 0.56              |
| 1:F:287:ILE:HG21 | 1:H:65:LEU:CD2   | 2.34                     | 0.56              |
| 1:G:242:LEU:CD1  | 1:G:243:PRO:HD2  | 2.35                     | 0.56              |
| 1:H:117:GLU:HA   | 1:H:367:PRO:CB   | 2.35                     | 0.56              |
| 1:H:250:ILE:HG13 | 1:H:253:GLU:HB2  | 1.87                     | 0.56              |
| 1:I:153:LEU:HD13 | 1:I:162:ASN:OD1  | 2.05                     | 0.56              |
| 1:I:166:TYR:CG   | 1:I:289:ILE:HG21 | 2.41                     | 0.56              |
| 1:I:169:TYR:CD2  | 1:I:375:PHE:HA   | 2.40                     | 0.56              |
| 1:I:250:ILE:HG13 | 1:I:253:GLU:HB2  | 1.87                     | 0.56              |
| 1:J:345:ILE:O    | 1:J:349:LEU:HG   | 2.05                     | 0.56              |
| 1:K:166:TYR:CG   | 1:K:289:ILE:HG21 | 2.41                     | 0.56              |
| 1:K:169:TYR:CD2  | 1:K:375:PHE:HA   | 2.40                     | 0.56              |
| 1:D:117:GLU:HA   | 1:D:367:PRO:CB   | 2.35                     | 0.56              |
| 1:D:153:LEU:HD13 | 1:D:162:ASN:OD1  | 2.05                     | 0.56              |
| 1:E:117:GLU:HA   | 1:E:367:PRO:CB   | 2.35                     | 0.56              |
| 1:E:139:VAL:HA   | 1:E:165:ILE:HD11 | 1.87                     | 0.56              |
| 1:E:242:LEU:CD1  | 1:E:243:PRO:HD2  | 2.35                     | 0.56              |
| 1:H:287:ILE:CG2  | 1:J:65:LEU:HD21  | 2.36                     | 0.56              |
| 1:H:345:ILE:O    | 1:H:349:LEU:HG   | 2.05                     | 0.56              |
| 1:J:169:TYR:CD2  | 1:J:375:PHE:HA   | 2.40                     | 0.56              |
| 1:A:153:LEU:HD13 | 1:A:162:ASN:OD1  | 2.05                     | 0.56              |
| 1:G:117:GLU:HA   | 1:G:367:PRO:CB   | 2.35                     | 0.56              |
| 1:K:35:VAL:CG2   | 1:K:81:ASP:HB3   | 2.34                     | 0.56              |
| 1:K:117:GLU:HA   | 1:K:367:PRO:CB   | 2.35                     | 0.56              |
| 1:C:169:TYR:CD2  | 1:C:375:PHE:HA   | 2.40                     | 0.56              |
| 1:C:345:ILE:O    | 1:C:349:LEU:HG   | 2.05                     | 0.56              |
| 1:E:153:LEU:HD13 | 1:E:162:ASN:OD1  | 2.05                     | 0.56              |
| 1:F:287:ILE:CG2  | 1:H:65:LEU:HD21  | 2.36                     | 0.56              |
| 1:I:345:ILE:O    | 1:I:349:LEU:HG   | 2.05                     | 0.56              |
| 1:J:117:GLU:HA   | 1:J:367:PRO:CB   | 2.35                     | 0.56              |
| 1:K:153:LEU:HD13 | 1:K:162:ASN:OD1  | 2.05                     | 0.56              |
| 1:A:242:LEU:CD1  | 1:A:243:PRO:HD2  | 2.35                     | 0.56              |
| 1:A:287:ILE:CG2  | 1:C:65:LEU:HD21  | 2.36                     | 0.56              |
| 1:C:287:ILE:CG2  | 1:E:65:LEU:HD21  | 2.36                     | 0.56              |
| 1:D:171:LEU:HD21 | 1:F:45:VAL:HG12  | 1.75                     | 0.56              |
| 1:D:345:ILE:O    | 1:D:349:LEU:HG   | 2.05                     | 0.56              |
| 1:G:169:TYR:CD2  | 1:G:375:PHE:HA   | 2.40                     | 0.56              |
| 1:H:169:TYR:CD2  | 1:H:375:PHE:HA   | 2.40                     | 0.56              |
| 1:B:166:TYR:CG   | 1:B:289:ILE:HG21 | 2.41                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:169:TYR:CD2  | 1:F:375:PHE:HA   | 2.40                     | 0.56              |
| 1:F:242:LEU:CD1  | 1:F:243:PRO:HD2  | 2.35                     | 0.56              |
| 1:I:117:GLU:HA   | 1:I:367:PRO:CB   | 2.35                     | 0.56              |
| 1:A:166:TYR:CG   | 1:A:289:ILE:HG21 | 2.41                     | 0.56              |
| 1:C:250:ILE:HG13 | 1:C:253:GLU:HB2  | 1.87                     | 0.56              |
| 1:F:345:ILE:O    | 1:F:349:LEU:HG   | 2.05                     | 0.56              |
| 1:I:35:VAL:CG2   | 1:I:81:ASP:HB3   | 2.34                     | 0.56              |
| 1:I:287:ILE:CG2  | 1:K:65:LEU:HD21  | 2.36                     | 0.56              |
| 1:J:153:LEU:HD13 | 1:J:162:ASN:OD1  | 2.05                     | 0.56              |
| 1:C:153:LEU:HD13 | 1:C:162:ASN:OD1  | 2.05                     | 0.56              |
| 1:D:169:TYR:CD2  | 1:D:375:PHE:HA   | 2.40                     | 0.56              |
| 1:G:153:LEU:HD13 | 1:G:162:ASN:OD1  | 2.05                     | 0.56              |
| 1:G:250:ILE:HG13 | 1:G:253:GLU:HB2  | 1.87                     | 0.56              |
| 1:H:287:ILE:HG21 | 1:J:65:LEU:CD2   | 2.34                     | 0.56              |
| 1:B:117:GLU:HA   | 1:B:367:PRO:CB   | 2.35                     | 0.55              |
| 1:B:218:TYR:O    | 1:B:255:PHE:HA   | 2.06                     | 0.55              |
| 1:C:35:VAL:CG2   | 1:C:81:ASP:HB3   | 2.34                     | 0.55              |
| 1:C:166:TYR:CG   | 1:C:289:ILE:HG21 | 2.41                     | 0.55              |
| 1:D:242:LEU:CD1  | 1:D:243:PRO:HD2  | 2.35                     | 0.55              |
| 1:D:286:ASP:HB2  | 1:F:46:GLY:O     | 2.07                     | 0.55              |
| 1:D:287:ILE:CG2  | 1:F:65:LEU:HD21  | 2.36                     | 0.55              |
| 1:E:287:ILE:CG2  | 1:G:65:LEU:HD21  | 2.36                     | 0.55              |
| 1:D:166:TYR:CG   | 1:D:289:ILE:HG21 | 2.41                     | 0.55              |
| 1:D:218:TYR:O    | 1:D:255:PHE:HA   | 2.06                     | 0.55              |
| 1:E:250:ILE:HG13 | 1:E:253:GLU:HB2  | 1.87                     | 0.55              |
| 1:G:71:ILE:HG22  | 1:G:73:HIS:H     | 1.72                     | 0.55              |
| 1:G:171:LEU:HD21 | 1:I:45:VAL:HG12  | 1.75                     | 0.55              |
| 1:G:345:ILE:O    | 1:G:349:LEU:HG   | 2.05                     | 0.55              |
| 1:H:242:LEU:CD1  | 1:H:243:PRO:HD2  | 2.35                     | 0.55              |
| 1:J:250:ILE:HG13 | 1:J:253:GLU:HB2  | 1.87                     | 0.55              |
| 1:A:218:TYR:O    | 1:A:255:PHE:HA   | 2.06                     | 0.55              |
| 1:A:250:ILE:HG13 | 1:A:253:GLU:HB2  | 1.87                     | 0.55              |
| 1:H:286:ASP:HB2  | 1:J:46:GLY:O     | 2.06                     | 0.55              |
| 1:B:169:TYR:CD2  | 1:B:375:PHE:HA   | 2.40                     | 0.55              |
| 1:E:169:TYR:CD2  | 1:E:375:PHE:HA   | 2.40                     | 0.55              |
| 1:F:166:TYR:CG   | 1:F:289:ILE:HG21 | 2.41                     | 0.55              |
| 1:G:242:LEU:HB3  | 1:G:244:ASP:OD2  | 2.07                     | 0.55              |
| 1:G:287:ILE:CG2  | 1:I:65:LEU:HD21  | 2.36                     | 0.55              |
| 1:B:287:ILE:CG2  | 1:D:65:LEU:HD21  | 2.36                     | 0.55              |
| 1:C:53:TYR:HD1   | 1:C:57:GLU:OE2   | 1.90                     | 0.55              |
| 1:E:53:TYR:HD1   | 1:E:57:GLU:OE2   | 1.90                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:53:TYR:HD1   | 1:F:57:GLU:OE2   | 1.90                     | 0.55              |
| 1:F:218:TYR:O    | 1:F:255:PHE:HA   | 2.06                     | 0.55              |
| 1:J:166:TYR:CG   | 1:J:289:ILE:HG21 | 2.41                     | 0.55              |
| 1:D:189:LEU:CD1  | 1:D:253:GLU:HB3  | 2.37                     | 0.55              |
| 1:E:218:TYR:O    | 1:E:255:PHE:HA   | 2.06                     | 0.55              |
| 1:F:242:LEU:HB3  | 1:F:244:ASP:OD2  | 2.07                     | 0.55              |
| 1:F:286:ASP:HB2  | 1:H:46:GLY:O     | 2.07                     | 0.55              |
| 1:H:153:LEU:HD13 | 1:H:162:ASN:OD1  | 2.05                     | 0.55              |
| 1:I:242:LEU:HB3  | 1:I:244:ASP:OD2  | 2.07                     | 0.55              |
| 1:K:218:TYR:O    | 1:K:255:PHE:HA   | 2.06                     | 0.55              |
| 1:E:71:ILE:HG22  | 1:E:73:HIS:H     | 1.72                     | 0.55              |
| 1:F:153:LEU:HD13 | 1:F:162:ASN:OD1  | 2.05                     | 0.55              |
| 1:F:189:LEU:CD1  | 1:F:253:GLU:HB3  | 2.37                     | 0.55              |
| 1:I:71:ILE:HG22  | 1:I:73:HIS:H     | 1.72                     | 0.55              |
| 1:A:180:LEU:HD13 | 1:A:267:ILE:HD13 | 1.89                     | 0.55              |
| 1:B:153:LEU:HD13 | 1:B:162:ASN:OD1  | 2.05                     | 0.55              |
| 1:B:189:LEU:CD1  | 1:B:253:GLU:HB3  | 2.37                     | 0.55              |
| 1:J:53:TYR:HD1   | 1:J:57:GLU:OE2   | 1.90                     | 0.55              |
| 1:K:242:LEU:CD1  | 1:K:243:PRO:HD2  | 2.35                     | 0.55              |
| 1:B:31:PHE:HZ    | 1:B:89:THR:HG1   | 1.54                     | 0.55              |
| 1:E:180:LEU:HD13 | 1:E:267:ILE:HD13 | 1.89                     | 0.55              |
| 1:G:180:LEU:HD13 | 1:G:267:ILE:HD13 | 1.89                     | 0.55              |
| 1:H:242:LEU:HB3  | 1:H:244:ASP:OD2  | 2.07                     | 0.55              |
| 1:K:53:TYR:HD1   | 1:K:57:GLU:OE2   | 1.90                     | 0.55              |
| 1:K:189:LEU:CD1  | 1:K:253:GLU:HB3  | 2.37                     | 0.55              |
| 1:A:53:TYR:HD1   | 1:A:57:GLU:OE2   | 1.90                     | 0.54              |
| 1:A:287:ILE:CG1  | 1:C:61:LYS:HB3   | 2.37                     | 0.54              |
| 1:B:171:LEU:HD21 | 1:D:45:VAL:HG12  | 1.76                     | 0.54              |
| 1:B:242:LEU:HB3  | 1:B:244:ASP:OD2  | 2.07                     | 0.54              |
| 1:C:180:LEU:HD13 | 1:C:267:ILE:HD13 | 1.89                     | 0.54              |
| 1:C:218:TYR:O    | 1:C:255:PHE:HA   | 2.06                     | 0.54              |
| 1:D:53:TYR:HD1   | 1:D:57:GLU:OE2   | 1.90                     | 0.54              |
| 1:F:353:GLN:HA   | 1:F:356:TRP:CD1  | 2.43                     | 0.54              |
| 1:G:53:TYR:HD1   | 1:G:57:GLU:OE2   | 1.90                     | 0.54              |
| 1:H:189:LEU:CD1  | 1:H:253:GLU:HB3  | 2.37                     | 0.54              |
| 1:A:189:LEU:CD1  | 1:A:253:GLU:HB3  | 2.37                     | 0.54              |
| 1:A:242:LEU:HB3  | 1:A:244:ASP:OD2  | 2.07                     | 0.54              |
| 1:D:33:SER:HG    | 1:D:85:ILE:HD13  | 1.70                     | 0.54              |
| 1:G:353:GLN:HA   | 1:G:356:TRP:CD1  | 2.43                     | 0.54              |
| 1:I:180:LEU:HD13 | 1:I:267:ILE:HD13 | 1.89                     | 0.54              |
| 1:I:189:LEU:CD1  | 1:I:253:GLU:HB3  | 2.37                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:242:LEU:CD1  | 1:B:243:PRO:HD2  | 2.35                     | 0.54              |
| 1:G:218:TYR:O    | 1:G:255:PHE:HA   | 2.06                     | 0.54              |
| 1:J:218:TYR:O    | 1:J:255:PHE:HA   | 2.06                     | 0.54              |
| 1:J:353:GLN:HA   | 1:J:356:TRP:CD1  | 2.42                     | 0.54              |
| 1:B:53:TYR:HD1   | 1:B:57:GLU:OE2   | 1.90                     | 0.54              |
| 1:B:353:GLN:HA   | 1:B:356:TRP:CD1  | 2.43                     | 0.54              |
| 1:C:287:ILE:CG1  | 1:E:61:LYS:HB3   | 2.37                     | 0.54              |
| 1:G:189:LEU:CD1  | 1:G:253:GLU:HB3  | 2.37                     | 0.54              |
| 1:H:166:TYR:CG   | 1:H:289:ILE:HG21 | 2.41                     | 0.54              |
| 1:I:171:LEU:HD21 | 1:K:45:VAL:HG12  | 1.76                     | 0.54              |
| 1:I:218:TYR:O    | 1:I:255:PHE:HA   | 2.06                     | 0.54              |
| 1:K:242:LEU:HB3  | 1:K:244:ASP:OD2  | 2.07                     | 0.54              |
| 1:K:353:GLN:HA   | 1:K:356:TRP:CD1  | 2.43                     | 0.54              |
| 1:A:353:GLN:HA   | 1:A:356:TRP:CD1  | 2.42                     | 0.54              |
| 1:B:286:ASP:HB2  | 1:D:46:GLY:O     | 2.06                     | 0.54              |
| 1:B:287:ILE:CG1  | 1:D:61:LYS:O     | 2.56                     | 0.54              |
| 1:C:242:LEU:HB3  | 1:C:244:ASP:OD2  | 2.07                     | 0.54              |
| 1:E:124:PHE:O    | 1:E:128:ASN:HA   | 2.08                     | 0.54              |
| 1:F:287:ILE:CG1  | 1:H:61:LYS:HB3   | 2.38                     | 0.54              |
| 1:H:218:TYR:O    | 1:H:255:PHE:HA   | 2.06                     | 0.54              |
| 1:A:124:PHE:O    | 1:A:128:ASN:HA   | 2.08                     | 0.54              |
| 1:C:71:ILE:HG22  | 1:C:73:HIS:H     | 1.72                     | 0.54              |
| 1:C:124:PHE:O    | 1:C:128:ASN:HA   | 2.08                     | 0.54              |
| 1:E:189:LEU:CD1  | 1:E:253:GLU:HB3  | 2.37                     | 0.54              |
| 1:E:242:LEU:HB3  | 1:E:244:ASP:OD2  | 2.07                     | 0.54              |
| 1:G:124:PHE:O    | 1:G:128:ASN:HA   | 2.08                     | 0.54              |
| 1:I:117:GLU:HA   | 1:I:367:PRO:CG   | 2.38                     | 0.54              |
| 1:J:180:LEU:HD13 | 1:J:267:ILE:HD13 | 1.89                     | 0.54              |
| 1:B:71:ILE:HG22  | 1:B:73:HIS:H     | 1.72                     | 0.54              |
| 1:C:189:LEU:CD1  | 1:C:253:GLU:HB3  | 2.37                     | 0.54              |
| 1:C:353:GLN:HA   | 1:C:356:TRP:CD1  | 2.42                     | 0.54              |
| 1:D:242:LEU:HB3  | 1:D:244:ASP:OD2  | 2.07                     | 0.54              |
| 1:D:287:ILE:CG1  | 1:F:61:LYS:HB3   | 2.38                     | 0.54              |
| 1:D:353:GLN:HA   | 1:D:356:TRP:CD1  | 2.43                     | 0.54              |
| 1:G:287:ILE:CG1  | 1:I:65:LEU:HG    | 2.35                     | 0.54              |
| 1:H:180:LEU:HD13 | 1:H:267:ILE:HD13 | 1.89                     | 0.54              |
| 1:H:287:ILE:CG1  | 1:J:61:LYS:HB3   | 2.37                     | 0.54              |
| 1:I:287:ILE:CG1  | 1:K:61:LYS:HB3   | 2.37                     | 0.54              |
| 1:J:124:PHE:O    | 1:J:128:ASN:HA   | 2.08                     | 0.54              |
| 1:J:242:LEU:HB3  | 1:J:244:ASP:OD2  | 2.07                     | 0.54              |
| 1:K:71:ILE:HG22  | 1:K:73:HIS:H     | 1.72                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:286:ASP:HB2  | 1:C:46:GLY:O     | 2.06                     | 0.54              |
| 1:A:287:ILE:CG1  | 1:C:61:LYS:O     | 2.56                     | 0.54              |
| 1:B:117:GLU:HA   | 1:B:367:PRO:CG   | 2.38                     | 0.54              |
| 1:C:117:GLU:HA   | 1:C:367:PRO:CG   | 2.38                     | 0.54              |
| 1:C:286:ASP:HB2  | 1:E:46:GLY:O     | 2.07                     | 0.54              |
| 1:D:287:ILE:CG1  | 1:F:61:LYS:O     | 2.56                     | 0.54              |
| 1:H:117:GLU:HA   | 1:H:367:PRO:CG   | 2.38                     | 0.54              |
| 1:J:117:GLU:HA   | 1:J:367:PRO:CG   | 2.38                     | 0.54              |
| 1:J:189:LEU:CD1  | 1:J:253:GLU:HB3  | 2.37                     | 0.54              |
| 1:K:180:LEU:HD13 | 1:K:267:ILE:HD13 | 1.89                     | 0.54              |
| 1:D:193:LEU:CD2  | 1:D:253:GLU:HG2  | 2.38                     | 0.54              |
| 1:E:287:ILE:CG1  | 1:G:61:LYS:HB3   | 2.38                     | 0.54              |
| 1:H:287:ILE:CG1  | 1:J:61:LYS:O     | 2.56                     | 0.54              |
| 1:I:53:TYR:HD1   | 1:I:57:GLU:OE2   | 1.90                     | 0.54              |
| 1:G:286:ASP:HB2  | 1:I:46:GLY:O     | 2.06                     | 0.54              |
| 1:I:286:ASP:HB2  | 1:K:46:GLY:O     | 2.06                     | 0.54              |
| 1:I:353:GLN:HA   | 1:I:356:TRP:CD1  | 2.43                     | 0.54              |
| 1:A:71:ILE:HG22  | 1:A:73:HIS:H     | 1.72                     | 0.53              |
| 1:D:117:GLU:HA   | 1:D:367:PRO:CG   | 2.38                     | 0.53              |
| 1:E:353:GLN:HA   | 1:E:356:TRP:CD1  | 2.43                     | 0.53              |
| 1:G:117:GLU:HA   | 1:G:367:PRO:CG   | 2.38                     | 0.53              |
| 1:I:124:PHE:O    | 1:I:128:ASN:HA   | 2.08                     | 0.53              |
| 1:J:193:LEU:CD2  | 1:J:253:GLU:HG2  | 2.38                     | 0.53              |
| 1:A:193:LEU:CD2  | 1:A:253:GLU:HG2  | 2.38                     | 0.53              |
| 1:D:71:ILE:HG22  | 1:D:73:HIS:H     | 1.72                     | 0.53              |
| 1:E:286:ASP:HB2  | 1:G:46:GLY:O     | 2.07                     | 0.53              |
| 1:E:287:ILE:CG1  | 1:G:65:LEU:HG    | 2.35                     | 0.53              |
| 1:F:193:LEU:CD2  | 1:F:253:GLU:HG2  | 2.38                     | 0.53              |
| 1:F:287:ILE:CG1  | 1:H:61:LYS:O     | 2.56                     | 0.53              |
| 1:I:172:PRO:HA   | 1:I:175:ILE:HD12 | 1.91                     | 0.53              |
| 1:I:287:ILE:CG1  | 1:K:61:LYS:O     | 2.56                     | 0.53              |
| 1:J:71:ILE:HG22  | 1:J:73:HIS:H     | 1.72                     | 0.53              |
| 1:A:117:GLU:HA   | 1:A:367:PRO:CG   | 2.38                     | 0.53              |
| 1:B:287:ILE:CG1  | 1:D:61:LYS:HB3   | 2.38                     | 0.53              |
| 1:E:172:PRO:HA   | 1:E:175:ILE:HD12 | 1.91                     | 0.53              |
| 1:F:180:LEU:HD13 | 1:F:267:ILE:HD13 | 1.89                     | 0.53              |
| 1:G:172:PRO:HA   | 1:G:175:ILE:HD12 | 1.91                     | 0.53              |
| 1:B:172:PRO:HA   | 1:B:175:ILE:HD12 | 1.91                     | 0.53              |
| 1:C:193:LEU:CD2  | 1:C:253:GLU:HG2  | 2.38                     | 0.53              |
| 1:G:287:ILE:CG1  | 1:I:61:LYS:HB3   | 2.38                     | 0.53              |
| 1:H:124:PHE:O    | 1:H:128:ASN:HA   | 2.08                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:353:GLN:HA   | 1:H:356:TRP:CD1  | 2.43                     | 0.53              |
| 1:I:192:ILE:HG13 | 1:I:253:GLU:HG3  | 1.91                     | 0.53              |
| 1:J:31:PHE:HZ    | 1:J:89:THR:HG1   | 1.55                     | 0.53              |
| 1:K:117:GLU:HA   | 1:K:367:PRO:CG   | 2.38                     | 0.53              |
| 1:K:172:PRO:HA   | 1:K:175:ILE:HD12 | 1.91                     | 0.53              |
| 1:B:180:LEU:HD13 | 1:B:267:ILE:HD13 | 1.89                     | 0.53              |
| 1:C:287:ILE:CG1  | 1:E:61:LYS:O     | 2.56                     | 0.53              |
| 1:E:117:GLU:HA   | 1:E:367:PRO:CG   | 2.38                     | 0.53              |
| 1:B:192:ILE:HG13 | 1:B:253:GLU:HG3  | 1.91                     | 0.53              |
| 1:B:287:ILE:CG1  | 1:D:65:LEU:HG    | 2.35                     | 0.53              |
| 1:E:287:ILE:CG1  | 1:G:61:LYS:O     | 2.56                     | 0.53              |
| 1:G:192:ILE:HG13 | 1:G:253:GLU:HG3  | 1.91                     | 0.53              |
| 1:H:53:TYR:HD1   | 1:H:57:GLU:OE2   | 1.90                     | 0.53              |
| 1:C:172:PRO:HA   | 1:C:175:ILE:HD12 | 1.91                     | 0.53              |
| 1:F:117:GLU:HA   | 1:F:367:PRO:CG   | 2.38                     | 0.53              |
| 1:I:54:VAL:HG21  | 1:I:84:LYS:HD3   | 1.91                     | 0.53              |
| 1:I:193:LEU:CD2  | 1:I:253:GLU:HG2  | 2.38                     | 0.53              |
| 1:J:8:LEU:HG     | 1:J:101:HIS:HB3  | 1.91                     | 0.53              |
| 1:K:54:VAL:HG21  | 1:K:84:LYS:HD3   | 1.91                     | 0.53              |
| 1:K:192:ILE:HG13 | 1:K:253:GLU:HG3  | 1.91                     | 0.53              |
| 1:D:172:PRO:HA   | 1:D:175:ILE:HD12 | 1.91                     | 0.53              |
| 1:D:180:LEU:HD13 | 1:D:267:ILE:HD13 | 1.89                     | 0.53              |
| 1:F:71:ILE:HG22  | 1:F:73:HIS:H     | 1.72                     | 0.53              |
| 1:G:219:VAL:HG21 | 1:G:312:ARG:HG2  | 1.91                     | 0.53              |
| 1:H:8:LEU:HG     | 1:H:101:HIS:HB3  | 1.91                     | 0.53              |
| 1:H:193:LEU:CD2  | 1:H:253:GLU:HG2  | 2.38                     | 0.53              |
| 1:I:219:VAL:HG21 | 1:I:312:ARG:HG2  | 1.91                     | 0.53              |
| 1:B:8:LEU:HG     | 1:B:101:HIS:HB3  | 1.91                     | 0.53              |
| 1:B:124:PHE:O    | 1:B:128:ASN:HA   | 2.08                     | 0.53              |
| 1:D:124:PHE:CZ   | 1:D:132:MET:HG3  | 2.44                     | 0.53              |
| 1:E:193:LEU:CD2  | 1:E:253:GLU:HG2  | 2.38                     | 0.53              |
| 1:G:193:LEU:CD2  | 1:G:253:GLU:HG2  | 2.38                     | 0.53              |
| 1:I:287:ILE:CG1  | 1:K:65:LEU:HG    | 2.36                     | 0.53              |
| 1:B:54:VAL:HG21  | 1:B:84:LYS:HD3   | 1.91                     | 0.53              |
| 1:B:124:PHE:CZ   | 1:B:132:MET:HG3  | 2.44                     | 0.53              |
| 1:D:8:LEU:HG     | 1:D:101:HIS:HB3  | 1.91                     | 0.53              |
| 1:E:219:VAL:HG21 | 1:E:312:ARG:HG2  | 1.91                     | 0.53              |
| 1:J:124:PHE:CZ   | 1:J:132:MET:HG3  | 2.44                     | 0.53              |
| 1:K:124:PHE:O    | 1:K:128:ASN:HA   | 2.08                     | 0.53              |
| 1:K:219:VAL:HG21 | 1:K:312:ARG:HG2  | 1.91                     | 0.53              |
| 1:A:124:PHE:CZ   | 1:A:132:MET:HG3  | 2.44                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:124:PHE:CZ   | 1:C:132:MET:HG3  | 2.44                     | 0.52              |
| 1:F:124:PHE:O    | 1:F:128:ASN:HA   | 2.08                     | 0.52              |
| 1:G:54:VAL:HG21  | 1:G:84:LYS:HD3   | 1.91                     | 0.52              |
| 1:G:287:ILE:CG1  | 1:I:61:LYS:O     | 2.56                     | 0.52              |
| 1:H:71:ILE:HG22  | 1:H:73:HIS:H     | 1.72                     | 0.52              |
| 1:A:172:PRO:HA   | 1:A:175:ILE:HD12 | 1.91                     | 0.52              |
| 1:B:193:LEU:CD2  | 1:B:253:GLU:HG2  | 2.38                     | 0.52              |
| 1:D:192:ILE:HG13 | 1:D:253:GLU:HG3  | 1.91                     | 0.52              |
| 1:E:124:PHE:CZ   | 1:E:132:MET:HG3  | 2.44                     | 0.52              |
| 1:F:8:LEU:HG     | 1:F:101:HIS:HB3  | 1.91                     | 0.52              |
| 1:H:44:MET:HA    | 1:H:47:MET:HG2   | 1.92                     | 0.52              |
| 1:C:219:VAL:HG21 | 1:C:312:ARG:HG2  | 1.91                     | 0.52              |
| 1:D:54:VAL:HG21  | 1:D:84:LYS:HD3   | 1.91                     | 0.52              |
| 1:D:287:ILE:CG1  | 1:F:65:LEU:HG    | 2.36                     | 0.52              |
| 1:G:44:MET:HA    | 1:G:47:MET:HG2   | 1.92                     | 0.52              |
| 1:I:44:MET:HA    | 1:I:47:MET:HG2   | 1.92                     | 0.52              |
| 1:K:193:LEU:CD2  | 1:K:253:GLU:HG2  | 2.38                     | 0.52              |
| 1:D:124:PHE:O    | 1:D:128:ASN:HA   | 2.08                     | 0.52              |
| 1:E:192:ILE:HG13 | 1:E:253:GLU:HG3  | 1.91                     | 0.52              |
| 1:F:172:PRO:HA   | 1:F:175:ILE:CD1  | 2.40                     | 0.52              |
| 1:F:192:ILE:HG13 | 1:F:253:GLU:HG3  | 1.91                     | 0.52              |
| 1:A:6:THR:O      | 1:A:102:PRO:HD2  | 2.10                     | 0.52              |
| 1:A:44:MET:HA    | 1:A:47:MET:HG2   | 1.92                     | 0.52              |
| 1:A:154:ASP:O    | 1:A:160:THR:HA   | 2.10                     | 0.52              |
| 1:A:172:PRO:HA   | 1:A:175:ILE:CD1  | 2.40                     | 0.52              |
| 1:A:219:VAL:HG21 | 1:A:312:ARG:HG2  | 1.91                     | 0.52              |
| 1:B:172:PRO:HA   | 1:B:175:ILE:CD1  | 2.40                     | 0.52              |
| 1:D:97:ALA:HB3   | 1:D:100:GLU:HG2  | 1.91                     | 0.52              |
| 1:E:154:ASP:O    | 1:E:160:THR:HA   | 2.10                     | 0.52              |
| 1:E:172:PRO:HA   | 1:E:175:ILE:CD1  | 2.40                     | 0.52              |
| 1:J:172:PRO:HA   | 1:J:175:ILE:CD1  | 2.40                     | 0.52              |
| 1:K:154:ASP:O    | 1:K:160:THR:HA   | 2.10                     | 0.52              |
| 1:A:8:LEU:HG     | 1:A:101:HIS:HB3  | 1.91                     | 0.52              |
| 1:B:97:ALA:HB3   | 1:B:100:GLU:HG2  | 1.91                     | 0.52              |
| 1:C:154:ASP:O    | 1:C:160:THR:HA   | 2.10                     | 0.52              |
| 1:E:44:MET:HA    | 1:E:47:MET:HG2   | 1.92                     | 0.52              |
| 1:E:287:ILE:HA   | 1:G:64:ILE:HD12  | 1.89                     | 0.52              |
| 1:F:44:MET:HA    | 1:F:47:MET:HG2   | 1.92                     | 0.52              |
| 1:G:124:PHE:CZ   | 1:G:132:MET:HG3  | 2.44                     | 0.52              |
| 1:H:124:PHE:CZ   | 1:H:132:MET:HG3  | 2.44                     | 0.52              |
| 1:J:44:MET:HA    | 1:J:47:MET:HG2   | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:192:ILE:HG13 | 1:A:253:GLU:HG3  | 1.91                     | 0.52              |
| 1:B:287:ILE:HA   | 1:D:64:ILE:HD12  | 1.89                     | 0.52              |
| 1:C:6:THR:O      | 1:C:102:PRO:HD2  | 2.10                     | 0.52              |
| 1:C:287:ILE:CG1  | 1:E:65:LEU:HG    | 2.36                     | 0.52              |
| 1:D:154:ASP:O    | 1:D:160:THR:HA   | 2.10                     | 0.52              |
| 1:E:6:THR:O      | 1:E:102:PRO:HD2  | 2.10                     | 0.52              |
| 1:E:54:VAL:HG21  | 1:E:84:LYS:HD3   | 1.91                     | 0.52              |
| 1:F:54:VAL:HG21  | 1:F:84:LYS:HD3   | 1.91                     | 0.52              |
| 1:F:172:PRO:HA   | 1:F:175:ILE:HD12 | 1.91                     | 0.52              |
| 1:G:154:ASP:O    | 1:G:160:THR:HA   | 2.10                     | 0.52              |
| 1:G:287:ILE:HA   | 1:I:64:ILE:HD12  | 1.89                     | 0.52              |
| 1:H:154:ASP:O    | 1:H:160:THR:HA   | 2.10                     | 0.52              |
| 1:I:287:ILE:HA   | 1:K:64:ILE:HD12  | 1.89                     | 0.52              |
| 1:K:8:LEU:HG     | 1:K:101:HIS:HB3  | 1.91                     | 0.52              |
| 1:C:44:MET:HA    | 1:C:47:MET:HG2   | 1.92                     | 0.52              |
| 1:E:237:GLU:OE2  | 1:E:251:GLY:HA3  | 2.10                     | 0.52              |
| 1:F:124:PHE:CZ   | 1:F:132:MET:HG3  | 2.44                     | 0.52              |
| 1:G:97:ALA:HB3   | 1:G:100:GLU:HG2  | 1.91                     | 0.52              |
| 1:H:6:THR:O      | 1:H:102:PRO:HD2  | 2.10                     | 0.52              |
| 1:I:237:GLU:OE2  | 1:I:251:GLY:HA3  | 2.10                     | 0.52              |
| 1:J:154:ASP:O    | 1:J:160:THR:HA   | 2.10                     | 0.52              |
| 1:J:192:ILE:HG13 | 1:J:253:GLU:HG3  | 1.91                     | 0.52              |
| 1:B:34:ILE:HD12  | 1:B:67:LEU:HD22  | 1.91                     | 0.52              |
| 1:C:192:ILE:HG13 | 1:C:253:GLU:HG3  | 1.90                     | 0.52              |
| 1:D:287:ILE:HA   | 1:F:64:ILE:HD12  | 1.89                     | 0.52              |
| 1:E:97:ALA:HB3   | 1:E:100:GLU:HG2  | 1.91                     | 0.52              |
| 1:I:154:ASP:O    | 1:I:160:THR:HA   | 2.10                     | 0.52              |
| 1:K:6:THR:O      | 1:K:102:PRO:HD2  | 2.10                     | 0.52              |
| 1:K:172:PRO:HA   | 1:K:175:ILE:CD1  | 2.40                     | 0.52              |
| 1:A:180:LEU:HD23 | 1:A:261:LEU:HA   | 1.92                     | 0.52              |
| 1:B:70:PRO:HG3   | 1:B:85:ILE:CD1   | 2.41                     | 0.52              |
| 1:C:8:LEU:HG     | 1:C:101:HIS:HB3  | 1.91                     | 0.52              |
| 1:F:6:THR:O      | 1:F:102:PRO:HD2  | 2.10                     | 0.52              |
| 1:F:97:ALA:HB3   | 1:F:100:GLU:HG2  | 1.91                     | 0.52              |
| 1:F:154:ASP:O    | 1:F:160:THR:HA   | 2.10                     | 0.52              |
| 1:H:192:ILE:HG13 | 1:H:253:GLU:HG3  | 1.91                     | 0.52              |
| 1:H:219:VAL:HG21 | 1:H:312:ARG:HG2  | 1.91                     | 0.52              |
| 1:H:237:GLU:OE2  | 1:H:251:GLY:HA3  | 2.10                     | 0.52              |
| 1:I:124:PHE:CZ   | 1:I:132:MET:HG3  | 2.44                     | 0.52              |
| 1:J:6:THR:O      | 1:J:102:PRO:HD2  | 2.10                     | 0.52              |
| 1:K:44:MET:HA    | 1:K:47:MET:HG2   | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:124:PHE:CZ   | 1:K:132:MET:HG3  | 2.44                     | 0.52              |
| 1:B:6:THR:O      | 1:B:102:PRO:HD2  | 2.10                     | 0.51              |
| 1:B:154:ASP:O    | 1:B:160:THR:HA   | 2.10                     | 0.51              |
| 1:D:248:ILE:HD13 | 1:D:248:ILE:N    | 2.25                     | 0.51              |
| 1:F:180:LEU:HD23 | 1:F:261:LEU:HA   | 1.92                     | 0.51              |
| 1:F:248:ILE:HD13 | 1:F:248:ILE:N    | 2.25                     | 0.51              |
| 1:G:6:THR:O      | 1:G:102:PRO:HD2  | 2.10                     | 0.51              |
| 1:H:70:PRO:HG3   | 1:H:85:ILE:CD1   | 2.41                     | 0.51              |
| 1:H:172:PRO:HA   | 1:H:175:ILE:CD1  | 2.40                     | 0.51              |
| 1:I:6:THR:O      | 1:I:102:PRO:HD2  | 2.10                     | 0.51              |
| 1:I:70:PRO:HG3   | 1:I:85:ILE:CD1   | 2.41                     | 0.51              |
| 1:J:34:ILE:HD12  | 1:J:67:LEU:HD22  | 1.91                     | 0.51              |
| 1:J:237:GLU:OE2  | 1:J:251:GLY:HA3  | 2.10                     | 0.51              |
| 1:K:117:GLU:HG2  | 1:K:367:PRO:HB2  | 1.92                     | 0.51              |
| 1:B:44:MET:HA    | 1:B:47:MET:HG2   | 1.92                     | 0.51              |
| 1:B:117:GLU:HG2  | 1:B:367:PRO:HB2  | 1.92                     | 0.51              |
| 1:B:219:VAL:HG21 | 1:B:312:ARG:HG2  | 1.91                     | 0.51              |
| 1:B:248:ILE:HD13 | 1:B:248:ILE:N    | 2.25                     | 0.51              |
| 1:D:44:MET:HA    | 1:D:47:MET:HG2   | 1.92                     | 0.51              |
| 1:F:219:VAL:HG21 | 1:F:312:ARG:HG2  | 1.91                     | 0.51              |
| 1:G:172:PRO:HA   | 1:G:175:ILE:CD1  | 2.40                     | 0.51              |
| 1:I:8:LEU:HG     | 1:I:101:HIS:HB3  | 1.91                     | 0.51              |
| 1:J:172:PRO:HA   | 1:J:175:ILE:HD12 | 1.91                     | 0.51              |
| 1:K:34:ILE:HD12  | 1:K:67:LEU:HD22  | 1.91                     | 0.51              |
| 1:A:34:ILE:HD12  | 1:A:67:LEU:HD22  | 1.91                     | 0.51              |
| 1:C:54:VAL:HG21  | 1:C:84:LYS:HD3   | 1.91                     | 0.51              |
| 1:C:172:PRO:HA   | 1:C:175:ILE:CD1  | 2.40                     | 0.51              |
| 1:C:180:LEU:HD23 | 1:C:261:LEU:HA   | 1.92                     | 0.51              |
| 1:C:237:GLU:OE2  | 1:C:251:GLY:HA3  | 2.10                     | 0.51              |
| 1:D:117:GLU:HG2  | 1:D:367:PRO:HB2  | 1.92                     | 0.51              |
| 1:D:268:GLY:HA3  | 1:E:40:HIS:HB3   | 1.93                     | 0.51              |
| 1:F:237:GLU:OE2  | 1:F:251:GLY:HA3  | 2.10                     | 0.51              |
| 1:F:268:GLY:HA3  | 1:G:40:HIS:HB3   | 1.93                     | 0.51              |
| 1:H:54:VAL:HG21  | 1:H:84:LYS:HD3   | 1.91                     | 0.51              |
| 1:I:97:ALA:HB3   | 1:I:100:GLU:HG2  | 1.92                     | 0.51              |
| 1:J:180:LEU:HD23 | 1:J:261:LEU:HA   | 1.92                     | 0.51              |
| 1:J:219:VAL:HG21 | 1:J:312:ARG:HG2  | 1.91                     | 0.51              |
| 1:K:97:ALA:HB3   | 1:K:100:GLU:HG2  | 1.91                     | 0.51              |
| 1:A:54:VAL:HG21  | 1:A:84:LYS:HD3   | 1.91                     | 0.51              |
| 1:A:97:ALA:HB3   | 1:A:100:GLU:HG2  | 1.91                     | 0.51              |
| 1:A:287:ILE:HA   | 1:C:64:ILE:HD12  | 1.89                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:268:GLY:HA3  | 1:C:40:HIS:HB3  | 1.93                     | 0.51              |
| 1:C:70:PRO:HG3   | 1:C:85:ILE:CD1  | 2.41                     | 0.51              |
| 1:D:6:THR:O      | 1:D:102:PRO:HD2 | 2.10                     | 0.51              |
| 1:D:34:ILE:HD12  | 1:D:67:LEU:HD22 | 1.91                     | 0.51              |
| 1:F:287:ILE:HA   | 1:H:64:ILE:HD12 | 1.89                     | 0.51              |
| 1:I:117:GLU:HG2  | 1:I:367:PRO:HB2 | 1.92                     | 0.51              |
| 1:I:172:PRO:HA   | 1:I:175:ILE:CD1 | 2.40                     | 0.51              |
| 1:A:70:PRO:HG3   | 1:A:85:ILE:CD1  | 2.41                     | 0.51              |
| 1:C:268:GLY:HA3  | 1:D:40:HIS:HB3  | 1.93                     | 0.51              |
| 1:D:70:PRO:HG3   | 1:D:85:ILE:CD1  | 2.40                     | 0.51              |
| 1:D:172:PRO:HA   | 1:D:175:ILE:CD1 | 2.40                     | 0.51              |
| 1:E:117:GLU:CB   | 1:E:367:PRO:HG2 | 2.41                     | 0.51              |
| 1:E:268:GLY:HA3  | 1:F:40:HIS:HB3  | 1.93                     | 0.51              |
| 1:F:117:GLU:HA   | 1:F:367:PRO:HG2 | 1.93                     | 0.51              |
| 1:G:117:GLU:HG2  | 1:G:367:PRO:HB2 | 1.92                     | 0.51              |
| 1:H:248:ILE:HD13 | 1:H:248:ILE:N   | 2.25                     | 0.51              |
| 1:H:268:GLY:HA3  | 1:I:40:HIS:HB3  | 1.93                     | 0.51              |
| 1:J:54:VAL:HG21  | 1:J:84:LYS:HD3  | 1.91                     | 0.51              |
| 1:J:97:ALA:HB3   | 1:J:100:GLU:HG2 | 1.91                     | 0.51              |
| 1:C:97:ALA:HB3   | 1:C:100:GLU:HG2 | 1.91                     | 0.51              |
| 1:C:117:GLU:HA   | 1:C:367:PRO:HG2 | 1.93                     | 0.51              |
| 1:C:117:GLU:CB   | 1:C:367:PRO:HG2 | 2.41                     | 0.51              |
| 1:D:117:GLU:HA   | 1:D:367:PRO:HG2 | 1.93                     | 0.51              |
| 1:D:219:VAL:HG21 | 1:D:312:ARG:HG2 | 1.91                     | 0.51              |
| 1:E:34:ILE:HD12  | 1:E:67:LEU:HD22 | 1.91                     | 0.51              |
| 1:F:117:GLU:HG2  | 1:F:367:PRO:HB2 | 1.92                     | 0.51              |
| 1:F:287:ILE:CG1  | 1:H:65:LEU:HG   | 2.36                     | 0.51              |
| 1:G:8:LEU:HG     | 1:G:101:HIS:HB3 | 1.91                     | 0.51              |
| 1:G:180:LEU:HD23 | 1:G:261:LEU:HA  | 1.92                     | 0.51              |
| 1:G:237:GLU:OE2  | 1:G:251:GLY:HA3 | 2.10                     | 0.51              |
| 1:H:180:LEU:HD23 | 1:H:261:LEU:HA  | 1.92                     | 0.51              |
| 1:J:117:GLU:HA   | 1:J:367:PRO:HG2 | 1.93                     | 0.51              |
| 1:K:70:PRO:HG3   | 1:K:85:ILE:CD1  | 2.41                     | 0.51              |
| 1:A:117:GLU:HA   | 1:A:367:PRO:HG2 | 1.93                     | 0.51              |
| 1:A:117:GLU:HG2  | 1:A:367:PRO:HB2 | 1.92                     | 0.51              |
| 1:A:268:GLY:HA3  | 1:B:40:HIS:HB3  | 1.93                     | 0.51              |
| 1:C:34:ILE:HD12  | 1:C:67:LEU:HD22 | 1.91                     | 0.51              |
| 1:C:117:GLU:HG2  | 1:C:367:PRO:HB2 | 1.92                     | 0.51              |
| 1:E:8:LEU:HG     | 1:E:101:HIS:HB3 | 1.91                     | 0.51              |
| 1:F:34:ILE:HD12  | 1:F:67:LEU:HD22 | 1.91                     | 0.51              |
| 1:G:117:GLU:CB   | 1:G:367:PRO:HG2 | 2.41                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:97:ALA:HB3   | 1:H:100:GLU:HG2  | 1.91                     | 0.51              |
| 1:A:117:GLU:CB   | 1:A:367:PRO:HG2  | 2.41                     | 0.51              |
| 1:A:237:GLU:OE2  | 1:A:251:GLY:HA3  | 2.10                     | 0.51              |
| 1:F:70:PRO:HG3   | 1:F:85:ILE:CD1   | 2.41                     | 0.51              |
| 1:G:34:ILE:HD12  | 1:G:67:LEU:HD22  | 1.91                     | 0.51              |
| 1:G:268:GLY:HA3  | 1:H:40:HIS:HB3   | 1.93                     | 0.51              |
| 1:H:34:ILE:HD12  | 1:H:67:LEU:HD22  | 1.91                     | 0.51              |
| 1:H:117:GLU:HG2  | 1:H:367:PRO:HB2  | 1.92                     | 0.51              |
| 1:K:117:GLU:HA   | 1:K:367:PRO:HG2  | 1.93                     | 0.51              |
| 1:B:117:GLU:HA   | 1:B:367:PRO:HG2  | 1.93                     | 0.51              |
| 1:D:237:GLU:OE2  | 1:D:251:GLY:HA3  | 2.10                     | 0.51              |
| 1:E:117:GLU:HA   | 1:E:367:PRO:HG2  | 1.93                     | 0.51              |
| 1:G:31:PHE:HZ    | 1:G:89:THR:HG1   | 1.59                     | 0.51              |
| 1:G:70:PRO:HG3   | 1:G:85:ILE:CD1   | 2.41                     | 0.51              |
| 1:H:287:ILE:HA   | 1:J:64:ILE:HD12  | 1.89                     | 0.51              |
| 1:I:34:ILE:HD12  | 1:I:67:LEU:HD22  | 1.91                     | 0.51              |
| 1:I:117:GLU:HA   | 1:I:367:PRO:HG2  | 1.93                     | 0.51              |
| 1:J:268:GLY:HA3  | 1:K:40:HIS:HB3   | 1.93                     | 0.51              |
| 1:H:117:GLU:HA   | 1:H:367:PRO:HG2  | 1.93                     | 0.51              |
| 1:I:268:GLY:HA3  | 1:J:40:HIS:HB3   | 1.93                     | 0.51              |
| 1:J:70:PRO:HG3   | 1:J:85:ILE:CD1   | 2.41                     | 0.51              |
| 1:J:117:GLU:HG2  | 1:J:367:PRO:HB2  | 1.92                     | 0.51              |
| 1:K:248:ILE:HD13 | 1:K:248:ILE:N    | 2.25                     | 0.51              |
| 1:B:180:LEU:HD23 | 1:B:261:LEU:HA   | 1.92                     | 0.50              |
| 1:B:237:GLU:OE2  | 1:B:251:GLY:HA3  | 2.10                     | 0.50              |
| 1:E:117:GLU:HG2  | 1:E:367:PRO:HB2  | 1.92                     | 0.50              |
| 1:G:117:GLU:HA   | 1:G:367:PRO:HG2  | 1.93                     | 0.50              |
| 1:H:172:PRO:HA   | 1:H:175:ILE:HD12 | 1.91                     | 0.50              |
| 1:J:117:GLU:CB   | 1:J:367:PRO:HG2  | 2.41                     | 0.50              |
| 1:A:196:ARG:HH21 | 1:A:252:ASN:ND2  | 2.10                     | 0.50              |
| 1:D:143:TYR:CE2  | 1:D:346:LEU:HD22 | 2.46                     | 0.50              |
| 1:D:180:LEU:HD23 | 1:D:261:LEU:HA   | 1.92                     | 0.50              |
| 1:E:70:PRO:HG3   | 1:E:85:ILE:CD1   | 2.41                     | 0.50              |
| 1:G:196:ARG:HH21 | 1:G:252:ASN:ND2  | 2.10                     | 0.50              |
| 1:I:117:GLU:CB   | 1:I:367:PRO:HG2  | 2.41                     | 0.50              |
| 1:K:237:GLU:OE2  | 1:K:251:GLY:HA3  | 2.10                     | 0.50              |
| 1:A:287:ILE:CG1  | 1:C:65:LEU:HG    | 2.35                     | 0.50              |
| 1:B:143:TYR:CE2  | 1:B:346:LEU:HD22 | 2.47                     | 0.50              |
| 1:H:196:ARG:HH21 | 1:H:252:ASN:ND2  | 2.10                     | 0.50              |
| 1:I:248:ILE:HD13 | 1:I:248:ILE:N    | 2.25                     | 0.50              |
| 1:K:180:LEU:HD23 | 1:K:261:LEU:HA   | 1.92                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:267:ILE:HD11 | 1:A:269:MET:SD   | 2.52                     | 0.50              |
| 1:I:262:PHE:O    | 1:I:273:GLY:HA3  | 2.12                     | 0.50              |
| 1:J:196:ARG:HH21 | 1:J:252:ASN:ND2  | 2.10                     | 0.50              |
| 1:C:196:ARG:HH21 | 1:C:252:ASN:ND2  | 2.10                     | 0.50              |
| 1:C:287:ILE:HA   | 1:E:64:ILE:HD12  | 1.89                     | 0.50              |
| 1:D:267:ILE:HD11 | 1:D:269:MET:SD   | 2.52                     | 0.50              |
| 1:D:286:ASP:CB   | 1:F:46:GLY:O     | 2.60                     | 0.50              |
| 1:D:295:ALA:O    | 1:D:330:ILE:HD11 | 2.12                     | 0.50              |
| 1:F:117:GLU:CB   | 1:F:367:PRO:HG2  | 2.41                     | 0.50              |
| 1:F:143:TYR:CE2  | 1:F:346:LEU:HD22 | 2.46                     | 0.50              |
| 1:J:282:ILE:HG21 | 1:J:294:TYR:CE2  | 2.47                     | 0.50              |
| 1:K:117:GLU:CB   | 1:K:367:PRO:HG2  | 2.41                     | 0.50              |
| 1:A:31:PHE:HZ    | 1:A:89:THR:HG1   | 1.59                     | 0.50              |
| 1:C:286:ASP:CB   | 1:E:46:GLY:O     | 2.60                     | 0.50              |
| 1:E:180:LEU:HD23 | 1:E:261:LEU:HA   | 1.92                     | 0.50              |
| 1:E:267:ILE:HD11 | 1:E:269:MET:SD   | 2.52                     | 0.50              |
| 1:E:286:ASP:CB   | 1:G:46:GLY:O     | 2.60                     | 0.50              |
| 1:F:267:ILE:HD11 | 1:F:269:MET:SD   | 2.52                     | 0.50              |
| 1:F:295:ALA:O    | 1:F:330:ILE:HD11 | 2.12                     | 0.50              |
| 1:H:117:GLU:CB   | 1:H:367:PRO:HG2  | 2.41                     | 0.50              |
| 1:I:196:ARG:HH21 | 1:I:252:ASN:ND2  | 2.10                     | 0.50              |
| 1:I:282:ILE:HG21 | 1:I:294:TYR:CE2  | 2.47                     | 0.50              |
| 1:J:143:TYR:CE2  | 1:J:346:LEU:HD22 | 2.46                     | 0.50              |
| 1:K:262:PHE:O    | 1:K:273:GLY:HA3  | 2.12                     | 0.50              |
| 1:K:267:ILE:HD11 | 1:K:269:MET:SD   | 2.52                     | 0.50              |
| 1:A:143:TYR:CE2  | 1:A:346:LEU:HD22 | 2.46                     | 0.50              |
| 1:B:286:ASP:CB   | 1:D:46:GLY:O     | 2.60                     | 0.50              |
| 1:C:262:PHE:O    | 1:C:273:GLY:HA3  | 2.12                     | 0.50              |
| 1:C:267:ILE:HD11 | 1:C:269:MET:SD   | 2.52                     | 0.50              |
| 1:E:196:ARG:HH21 | 1:E:252:ASN:ND2  | 2.10                     | 0.50              |
| 1:F:290:ARG:CD   | 1:H:64:ILE:HD13  | 2.38                     | 0.50              |
| 1:G:248:ILE:HD13 | 1:G:248:ILE:N    | 2.25                     | 0.50              |
| 1:H:143:TYR:CE2  | 1:H:346:LEU:HD22 | 2.47                     | 0.50              |
| 1:H:267:ILE:HD11 | 1:H:269:MET:SD   | 2.52                     | 0.50              |
| 1:H:286:ASP:CB   | 1:J:46:GLY:O     | 2.60                     | 0.50              |
| 1:J:122:ILE:O    | 1:J:126:THR:HB   | 2.12                     | 0.50              |
| 1:J:267:ILE:HD11 | 1:J:269:MET:SD   | 2.52                     | 0.50              |
| 1:K:143:TYR:CE2  | 1:K:346:LEU:HD22 | 2.46                     | 0.50              |
| 1:C:143:TYR:CE2  | 1:C:346:LEU:HD22 | 2.46                     | 0.50              |
| 1:E:262:PHE:O    | 1:E:273:GLY:HA3  | 2.12                     | 0.50              |
| 1:F:122:ILE:O    | 1:F:126:THR:HB   | 2.12                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:196:ARG:HH21 | 1:F:252:ASN:ND2  | 2.10                     | 0.50              |
| 1:I:267:ILE:HD11 | 1:I:269:MET:SD   | 2.52                     | 0.50              |
| 1:J:248:ILE:HD13 | 1:J:248:ILE:N    | 2.25                     | 0.50              |
| 1:K:295:ALA:O    | 1:K:330:ILE:HD11 | 2.12                     | 0.50              |
| 1:A:122:ILE:O    | 1:A:126:THR:HB   | 2.12                     | 0.50              |
| 1:B:117:GLU:CB   | 1:B:367:PRO:HG2  | 2.41                     | 0.50              |
| 1:B:267:ILE:HD11 | 1:B:269:MET:SD   | 2.52                     | 0.50              |
| 1:B:295:ALA:O    | 1:B:330:ILE:HD11 | 2.12                     | 0.50              |
| 1:E:143:TYR:CE2  | 1:E:346:LEU:HD22 | 2.46                     | 0.50              |
| 1:E:295:ALA:O    | 1:E:330:ILE:HD11 | 2.12                     | 0.50              |
| 1:F:282:ILE:HG21 | 1:F:294:TYR:CE2  | 2.47                     | 0.50              |
| 1:F:370:VAL:HG23 | 1:F:374:CYS:SG   | 2.52                     | 0.50              |
| 1:G:262:PHE:O    | 1:G:273:GLY:HA3  | 2.12                     | 0.50              |
| 1:I:295:ALA:O    | 1:I:330:ILE:HD11 | 2.12                     | 0.50              |
| 1:A:286:ASP:CB   | 1:C:46:GLY:O     | 2.60                     | 0.49              |
| 1:B:122:ILE:O    | 1:B:126:THR:HB   | 2.12                     | 0.49              |
| 1:G:143:TYR:CE2  | 1:G:346:LEU:HD22 | 2.46                     | 0.49              |
| 1:G:282:ILE:HG21 | 1:G:294:TYR:CE2  | 2.47                     | 0.49              |
| 1:G:286:ASP:CB   | 1:I:46:GLY:O     | 2.60                     | 0.49              |
| 1:G:295:ALA:O    | 1:G:330:ILE:HD11 | 2.12                     | 0.49              |
| 1:I:31:PHE:HZ    | 1:I:89:THR:HG1   | 1.59                     | 0.49              |
| 1:K:196:ARG:HH21 | 1:K:252:ASN:ND2  | 2.10                     | 0.49              |
| 1:C:295:ALA:O    | 1:C:330:ILE:HD11 | 2.12                     | 0.49              |
| 1:C:370:VAL:HG23 | 1:C:374:CYS:SG   | 2.52                     | 0.49              |
| 1:E:248:ILE:HD13 | 1:E:248:ILE:N    | 2.25                     | 0.49              |
| 1:H:287:ILE:CG1  | 1:J:65:LEU:HG    | 2.35                     | 0.49              |
| 1:H:295:ALA:O    | 1:H:330:ILE:HD11 | 2.12                     | 0.49              |
| 1:H:370:VAL:HG23 | 1:H:374:CYS:SG   | 2.52                     | 0.49              |
| 1:I:180:LEU:HD23 | 1:I:261:LEU:HA   | 1.92                     | 0.49              |
| 1:K:282:ILE:HG21 | 1:K:294:TYR:CE2  | 2.47                     | 0.49              |
| 1:A:370:VAL:HG23 | 1:A:374:CYS:SG   | 2.52                     | 0.49              |
| 1:I:143:TYR:CE2  | 1:I:346:LEU:HD22 | 2.46                     | 0.49              |
| 1:D:117:GLU:CB   | 1:D:367:PRO:HG2  | 2.41                     | 0.49              |
| 1:D:262:PHE:O    | 1:D:273:GLY:HA3  | 2.12                     | 0.49              |
| 1:E:370:VAL:HG23 | 1:E:374:CYS:SG   | 2.52                     | 0.49              |
| 1:F:286:ASP:CB   | 1:H:46:GLY:O     | 2.60                     | 0.49              |
| 1:A:190:MET:SD   | 1:A:206:ARG:HG3  | 2.53                     | 0.49              |
| 1:A:262:PHE:O    | 1:A:273:GLY:HA3  | 2.12                     | 0.49              |
| 1:A:282:ILE:HG21 | 1:A:294:TYR:CE2  | 2.47                     | 0.49              |
| 1:C:248:ILE:HD13 | 1:C:248:ILE:N    | 2.25                     | 0.49              |
| 1:D:370:VAL:HG23 | 1:D:374:CYS:SG   | 2.53                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:190:MET:SD   | 1:E:206:ARG:HG3  | 2.53                     | 0.49              |
| 1:F:262:PHE:O    | 1:F:273:GLY:HA3  | 2.12                     | 0.49              |
| 1:G:190:MET:SD   | 1:G:206:ARG:HG3  | 2.53                     | 0.49              |
| 1:J:370:VAL:HG23 | 1:J:374:CYS:SG   | 2.52                     | 0.49              |
| 1:K:190:MET:SD   | 1:K:206:ARG:HG3  | 2.53                     | 0.49              |
| 1:K:208:ILE:O    | 1:K:212:ILE:HG13 | 2.13                     | 0.49              |
| 1:K:370:VAL:HG23 | 1:K:374:CYS:SG   | 2.52                     | 0.49              |
| 1:B:208:ILE:O    | 1:B:212:ILE:HG13 | 2.13                     | 0.49              |
| 1:B:282:ILE:HG21 | 1:B:294:TYR:CE2  | 2.47                     | 0.49              |
| 1:D:196:ARG:HH21 | 1:D:252:ASN:ND2  | 2.10                     | 0.49              |
| 1:G:208:ILE:O    | 1:G:212:ILE:HG13 | 2.13                     | 0.49              |
| 1:H:262:PHE:O    | 1:H:273:GLY:HA3  | 2.12                     | 0.49              |
| 1:K:122:ILE:O    | 1:K:126:THR:HB   | 2.12                     | 0.49              |
| 1:A:248:ILE:HD13 | 1:A:248:ILE:N    | 2.25                     | 0.49              |
| 1:B:196:ARG:HH21 | 1:B:252:ASN:ND2  | 2.10                     | 0.49              |
| 1:C:282:ILE:O    | 1:C:285:CYS:HB2  | 2.13                     | 0.49              |
| 1:E:282:ILE:HG21 | 1:E:294:TYR:CE2  | 2.47                     | 0.49              |
| 1:G:370:VAL:HG23 | 1:G:374:CYS:SG   | 2.52                     | 0.49              |
| 1:H:122:ILE:O    | 1:H:126:THR:HB   | 2.12                     | 0.49              |
| 1:H:282:ILE:HG21 | 1:H:294:TYR:CE2  | 2.47                     | 0.49              |
| 1:J:262:PHE:O    | 1:J:273:GLY:HA3  | 2.12                     | 0.49              |
| 1:A:295:ALA:O    | 1:A:330:ILE:HD11 | 2.12                     | 0.49              |
| 1:B:262:PHE:O    | 1:B:273:GLY:HA3  | 2.12                     | 0.49              |
| 1:B:370:VAL:HG23 | 1:B:374:CYS:SG   | 2.52                     | 0.49              |
| 1:D:122:ILE:O    | 1:D:126:THR:HB   | 2.12                     | 0.49              |
| 1:D:143:TYR:HB2  | 1:D:342:GLY:CA   | 2.43                     | 0.49              |
| 1:I:122:ILE:O    | 1:I:126:THR:HB   | 2.12                     | 0.49              |
| 1:I:282:ILE:O    | 1:I:285:CYS:HB2  | 2.13                     | 0.49              |
| 1:A:173:HIS:CE1  | 1:C:45:VAL:HG21  | 2.48                     | 0.49              |
| 1:A:282:ILE:O    | 1:A:285:CYS:HB2  | 2.13                     | 0.49              |
| 1:D:17:VAL:CG2   | 1:D:33:SER:HB2   | 2.43                     | 0.49              |
| 1:D:124:PHE:CD1  | 1:D:359:LYS:HD3  | 2.48                     | 0.49              |
| 1:D:173:HIS:CE1  | 1:F:45:VAL:HG21  | 2.48                     | 0.49              |
| 1:D:282:ILE:HG21 | 1:D:294:TYR:CE2  | 2.47                     | 0.49              |
| 1:E:143:TYR:HB2  | 1:E:342:GLY:CA   | 2.43                     | 0.49              |
| 1:E:282:ILE:O    | 1:E:285:CYS:HB2  | 2.13                     | 0.49              |
| 1:G:17:VAL:CG2   | 1:G:33:SER:HB2   | 2.43                     | 0.49              |
| 1:G:267:ILE:HD11 | 1:G:269:MET:SD   | 2.52                     | 0.49              |
| 1:I:190:MET:SD   | 1:I:206:ARG:HG3  | 2.53                     | 0.49              |
| 1:J:282:ILE:O    | 1:J:285:CYS:HB2  | 2.13                     | 0.49              |
| 1:B:17:VAL:CG2   | 1:B:33:SER:HB2   | 2.43                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:124:PHE:CD1  | 1:B:359:LYS:HD3  | 2.48                     | 0.49              |
| 1:C:143:TYR:HB2  | 1:C:342:GLY:CA   | 2.43                     | 0.49              |
| 1:D:208:ILE:O    | 1:D:212:ILE:HG13 | 2.13                     | 0.49              |
| 1:E:122:ILE:O    | 1:E:126:THR:HB   | 2.12                     | 0.49              |
| 1:F:17:VAL:CG2   | 1:F:33:SER:HB2   | 2.43                     | 0.49              |
| 1:F:143:TYR:HB2  | 1:F:342:GLY:CA   | 2.43                     | 0.49              |
| 1:G:223:PHE:CE1  | 1:G:259:GLU:HG2  | 2.48                     | 0.49              |
| 1:H:124:PHE:CD1  | 1:H:359:LYS:HD3  | 2.48                     | 0.49              |
| 1:H:143:TYR:HB2  | 1:H:342:GLY:CA   | 2.43                     | 0.49              |
| 1:I:17:VAL:CG2   | 1:I:33:SER:HB2   | 2.43                     | 0.49              |
| 1:I:141:SER:OG   | 1:I:339:VAL:HG22 | 2.13                     | 0.49              |
| 1:I:223:PHE:CE1  | 1:I:259:GLU:HG2  | 2.48                     | 0.49              |
| 1:I:286:ASP:CB   | 1:K:46:GLY:O     | 2.60                     | 0.49              |
| 1:J:143:TYR:HB2  | 1:J:342:GLY:CA   | 2.43                     | 0.49              |
| 1:J:295:ALA:O    | 1:J:330:ILE:HD11 | 2.12                     | 0.49              |
| 1:K:141:SER:OG   | 1:K:339:VAL:HG22 | 2.13                     | 0.49              |
| 1:B:143:TYR:HB2  | 1:B:342:GLY:CA   | 2.43                     | 0.48              |
| 1:B:173:HIS:CE1  | 1:D:45:VAL:HG21  | 2.48                     | 0.48              |
| 1:B:223:PHE:CE1  | 1:B:259:GLU:HG2  | 2.48                     | 0.48              |
| 1:E:223:PHE:CE1  | 1:E:259:GLU:HG2  | 2.48                     | 0.48              |
| 1:F:124:PHE:CD1  | 1:F:359:LYS:HD3  | 2.48                     | 0.48              |
| 1:G:143:TYR:HB2  | 1:G:342:GLY:CA   | 2.43                     | 0.48              |
| 1:H:17:VAL:CG2   | 1:H:33:SER:HB2   | 2.43                     | 0.48              |
| 1:J:124:PHE:CD1  | 1:J:359:LYS:HD3  | 2.48                     | 0.48              |
| 1:K:223:PHE:CE1  | 1:K:259:GLU:HG2  | 2.48                     | 0.48              |
| 1:A:260:THR:HG21 | 1:A:267:ILE:CG2  | 2.43                     | 0.48              |
| 1:B:36:GLY:O     | 1:B:52:SER:HB2   | 2.14                     | 0.48              |
| 1:C:141:SER:OG   | 1:C:339:VAL:HG22 | 2.13                     | 0.48              |
| 1:C:173:HIS:CE1  | 1:E:45:VAL:HG21  | 2.48                     | 0.48              |
| 1:E:208:ILE:O    | 1:E:212:ILE:HG13 | 2.13                     | 0.48              |
| 1:F:141:SER:OG   | 1:F:339:VAL:HG22 | 2.13                     | 0.48              |
| 1:F:173:HIS:CE1  | 1:H:45:VAL:HG21  | 2.48                     | 0.48              |
| 1:G:124:PHE:CD1  | 1:G:359:LYS:HD3  | 2.48                     | 0.48              |
| 1:H:141:SER:OG   | 1:H:339:VAL:HG22 | 2.13                     | 0.48              |
| 1:I:143:TYR:HB2  | 1:I:342:GLY:CA   | 2.43                     | 0.48              |
| 1:I:370:VAL:HG23 | 1:I:374:CYS:SG   | 2.52                     | 0.48              |
| 1:K:124:PHE:CD1  | 1:K:359:LYS:HD3  | 2.48                     | 0.48              |
| 1:A:124:PHE:CD1  | 1:A:359:LYS:HD3  | 2.48                     | 0.48              |
| 1:A:141:SER:OG   | 1:A:339:VAL:HG22 | 2.13                     | 0.48              |
| 1:B:141:SER:OG   | 1:B:339:VAL:HG22 | 2.13                     | 0.48              |
| 1:C:36:GLY:O     | 1:C:52:SER:HB2   | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:124:PHE:CD1  | 1:C:359:LYS:HD3  | 2.48                     | 0.48              |
| 1:E:36:GLY:O     | 1:E:52:SER:HB2   | 2.14                     | 0.48              |
| 1:E:124:PHE:CD1  | 1:E:359:LYS:HD3  | 2.48                     | 0.48              |
| 1:E:173:HIS:CE1  | 1:G:45:VAL:HG21  | 2.48                     | 0.48              |
| 1:G:193:LEU:HD13 | 1:G:200:PHE:CE2  | 2.49                     | 0.48              |
| 1:G:282:ILE:O    | 1:G:285:CYS:HB2  | 2.13                     | 0.48              |
| 1:H:282:ILE:O    | 1:H:285:CYS:HB2  | 2.13                     | 0.48              |
| 1:I:124:PHE:CD1  | 1:I:359:LYS:HD3  | 2.48                     | 0.48              |
| 1:K:17:VAL:CG2   | 1:K:33:SER:HB2   | 2.43                     | 0.48              |
| 1:A:36:GLY:O     | 1:A:52:SER:HB2   | 2.14                     | 0.48              |
| 1:A:143:TYR:HB2  | 1:A:342:GLY:CA   | 2.43                     | 0.48              |
| 1:A:193:LEU:HD13 | 1:A:200:PHE:CE2  | 2.49                     | 0.48              |
| 1:A:208:ILE:O    | 1:A:212:ILE:HG13 | 2.13                     | 0.48              |
| 1:C:260:THR:HG21 | 1:C:267:ILE:CG2  | 2.43                     | 0.48              |
| 1:C:282:ILE:HG21 | 1:C:294:TYR:CE2  | 2.47                     | 0.48              |
| 1:D:36:GLY:O     | 1:D:52:SER:HB2   | 2.14                     | 0.48              |
| 1:D:141:SER:OG   | 1:D:339:VAL:HG22 | 2.13                     | 0.48              |
| 1:E:193:LEU:HD13 | 1:E:200:PHE:CE2  | 2.49                     | 0.48              |
| 1:E:260:THR:HG21 | 1:E:267:ILE:CG2  | 2.43                     | 0.48              |
| 1:F:208:ILE:O    | 1:F:212:ILE:HG13 | 2.13                     | 0.48              |
| 1:G:122:ILE:O    | 1:G:126:THR:HB   | 2.12                     | 0.48              |
| 1:H:190:MET:SD   | 1:H:206:ARG:HG3  | 2.53                     | 0.48              |
| 1:C:208:ILE:O    | 1:C:212:ILE:HG13 | 2.13                     | 0.48              |
| 1:E:17:VAL:CG2   | 1:E:33:SER:HB2   | 2.43                     | 0.48              |
| 1:F:36:GLY:O     | 1:F:52:SER:HB2   | 2.14                     | 0.48              |
| 1:G:141:SER:OG   | 1:G:339:VAL:HG22 | 2.13                     | 0.48              |
| 1:G:260:THR:HG21 | 1:G:267:ILE:CG2  | 2.43                     | 0.48              |
| 1:I:335:ARG:HA   | 1:I:338:SER:HG   | 1.78                     | 0.48              |
| 1:B:216:LEU:HD11 | 1:B:240:TYR:HB2  | 1.95                     | 0.48              |
| 1:B:282:ILE:O    | 1:B:285:CYS:HB2  | 2.13                     | 0.48              |
| 1:C:122:ILE:O    | 1:C:126:THR:HB   | 2.12                     | 0.48              |
| 1:C:190:MET:SD   | 1:C:206:ARG:HG3  | 2.53                     | 0.48              |
| 1:C:223:PHE:CE1  | 1:C:259:GLU:HG2  | 2.48                     | 0.48              |
| 1:D:282:ILE:O    | 1:D:285:CYS:HB2  | 2.13                     | 0.48              |
| 1:H:173:HIS:CE1  | 1:J:45:VAL:HG21  | 2.48                     | 0.48              |
| 1:I:193:LEU:HD13 | 1:I:200:PHE:CE2  | 2.49                     | 0.48              |
| 1:I:208:ILE:O    | 1:I:212:ILE:HG13 | 2.13                     | 0.48              |
| 1:J:193:LEU:HD13 | 1:J:200:PHE:CE2  | 2.49                     | 0.48              |
| 1:K:143:TYR:HB2  | 1:K:342:GLY:CA   | 2.43                     | 0.48              |
| 1:B:189:LEU:HD11 | 1:B:253:GLU:HB3  | 1.95                     | 0.48              |
| 1:B:190:MET:SD   | 1:B:206:ARG:HG3  | 2.53                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:193:LEU:HD13 | 1:C:200:PHE:CE2  | 2.49                     | 0.48              |
| 1:G:36:GLY:O     | 1:G:52:SER:HB2   | 2.14                     | 0.48              |
| 1:G:173:HIS:CE1  | 1:I:45:VAL:HG21  | 2.48                     | 0.48              |
| 1:H:36:GLY:O     | 1:H:52:SER:HB2   | 2.14                     | 0.48              |
| 1:J:17:VAL:CG2   | 1:J:33:SER:HB2   | 2.43                     | 0.48              |
| 1:J:260:THR:HG21 | 1:J:267:ILE:CG2  | 2.43                     | 0.48              |
| 1:K:139:VAL:HG11 | 1:K:375:PHE:CE2  | 2.49                     | 0.48              |
| 1:K:216:LEU:HD11 | 1:K:240:TYR:HB2  | 1.95                     | 0.48              |
| 1:C:216:LEU:HD11 | 1:C:240:TYR:HB2  | 1.95                     | 0.48              |
| 1:D:216:LEU:HD11 | 1:D:240:TYR:HB2  | 1.95                     | 0.48              |
| 1:D:223:PHE:CE1  | 1:D:259:GLU:HG2  | 2.49                     | 0.48              |
| 1:F:282:ILE:O    | 1:F:285:CYS:HB2  | 2.13                     | 0.48              |
| 1:G:90:PHE:HA    | 1:G:94:LEU:HD12  | 1.96                     | 0.48              |
| 1:H:113:LYS:HD3  | 1:H:113:LYS:N    | 2.29                     | 0.48              |
| 1:H:193:LEU:HD13 | 1:H:200:PHE:CE2  | 2.49                     | 0.48              |
| 1:H:223:PHE:CE1  | 1:H:259:GLU:HG2  | 2.48                     | 0.48              |
| 1:I:36:GLY:O     | 1:I:52:SER:HB2   | 2.14                     | 0.48              |
| 1:I:139:VAL:HG11 | 1:I:375:PHE:CE2  | 2.49                     | 0.48              |
| 1:I:207:GLU:O    | 1:I:210:ARG:HB3  | 2.14                     | 0.48              |
| 1:J:36:GLY:O     | 1:J:52:SER:HB2   | 2.14                     | 0.48              |
| 1:J:208:ILE:O    | 1:J:212:ILE:HG13 | 2.12                     | 0.48              |
| 1:K:282:ILE:O    | 1:K:285:CYS:HB2  | 2.13                     | 0.48              |
| 1:A:90:PHE:HA    | 1:A:94:LEU:HD12  | 1.96                     | 0.48              |
| 1:A:189:LEU:HD11 | 1:A:253:GLU:HB3  | 1.95                     | 0.48              |
| 1:C:17:VAL:CG2   | 1:C:33:SER:HB2   | 2.43                     | 0.48              |
| 1:C:189:LEU:HD11 | 1:C:253:GLU:HB3  | 1.95                     | 0.48              |
| 1:D:139:VAL:HG11 | 1:D:375:PHE:CE2  | 2.49                     | 0.48              |
| 1:E:216:LEU:HD11 | 1:E:240:TYR:HB2  | 1.95                     | 0.48              |
| 1:F:139:VAL:HG11 | 1:F:375:PHE:CE2  | 2.49                     | 0.48              |
| 1:F:190:MET:SD   | 1:F:206:ARG:HG3  | 2.53                     | 0.48              |
| 1:H:208:ILE:O    | 1:H:212:ILE:HG13 | 2.13                     | 0.48              |
| 1:J:216:LEU:HD11 | 1:J:240:TYR:HB2  | 1.95                     | 0.48              |
| 1:J:223:PHE:CE1  | 1:J:259:GLU:HG2  | 2.48                     | 0.48              |
| 1:K:90:PHE:HA    | 1:K:94:LEU:HD12  | 1.96                     | 0.48              |
| 1:A:17:VAL:CG2   | 1:A:33:SER:HB2   | 2.43                     | 0.47              |
| 1:B:139:VAL:HG11 | 1:B:375:PHE:CE2  | 2.49                     | 0.47              |
| 1:B:207:GLU:O    | 1:B:210:ARG:HB3  | 2.14                     | 0.47              |
| 1:C:196:ARG:HH22 | 1:C:231:ALA:HA   | 1.79                     | 0.47              |
| 1:D:190:MET:SD   | 1:D:206:ARG:HG3  | 2.53                     | 0.47              |
| 1:E:139:VAL:HG11 | 1:E:375:PHE:CE2  | 2.49                     | 0.47              |
| 1:E:189:LEU:HD11 | 1:E:253:GLU:HB3  | 1.95                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:90:PHE:HA    | 1:F:94:LEU:HD12  | 1.96                     | 0.47              |
| 1:F:260:THR:HG21 | 1:F:267:ILE:CG2  | 2.43                     | 0.47              |
| 1:G:139:VAL:HG11 | 1:G:375:PHE:CE2  | 2.49                     | 0.47              |
| 1:H:31:PHE:HZ    | 1:H:89:THR:HG1   | 1.60                     | 0.47              |
| 1:K:36:GLY:O     | 1:K:52:SER:HB2   | 2.14                     | 0.47              |
| 1:B:260:THR:HG21 | 1:B:267:ILE:CG2  | 2.43                     | 0.47              |
| 1:D:90:PHE:HA    | 1:D:94:LEU:HD12  | 1.96                     | 0.47              |
| 1:D:207:GLU:O    | 1:D:210:ARG:HB3  | 2.14                     | 0.47              |
| 1:E:113:LYS:HD3  | 1:E:113:LYS:N    | 2.29                     | 0.47              |
| 1:E:207:GLU:O    | 1:E:210:ARG:HB3  | 2.14                     | 0.47              |
| 1:F:223:PHE:CE1  | 1:F:259:GLU:HG2  | 2.48                     | 0.47              |
| 1:G:189:LEU:HD11 | 1:G:253:GLU:HB3  | 1.95                     | 0.47              |
| 1:H:139:VAL:HG11 | 1:H:375:PHE:CE2  | 2.49                     | 0.47              |
| 1:I:173:HIS:CE1  | 1:K:45:VAL:HG21  | 2.48                     | 0.47              |
| 1:J:190:MET:SD   | 1:J:206:ARG:HG3  | 2.53                     | 0.47              |
| 1:D:260:THR:HG21 | 1:D:267:ILE:CG2  | 2.43                     | 0.47              |
| 1:F:193:LEU:HD13 | 1:F:200:PHE:CE2  | 2.49                     | 0.47              |
| 1:F:216:LEU:HD11 | 1:F:240:TYR:HB2  | 1.95                     | 0.47              |
| 1:G:113:LYS:HD3  | 1:G:113:LYS:N    | 2.29                     | 0.47              |
| 1:H:260:THR:HG21 | 1:H:267:ILE:CG2  | 2.43                     | 0.47              |
| 1:I:216:LEU:HD11 | 1:I:240:TYR:HB2  | 1.95                     | 0.47              |
| 1:I:260:THR:HG21 | 1:I:267:ILE:CG2  | 2.43                     | 0.47              |
| 1:J:139:VAL:HG11 | 1:J:375:PHE:CE2  | 2.49                     | 0.47              |
| 1:B:113:LYS:HD3  | 1:B:113:LYS:N    | 2.29                     | 0.47              |
| 1:B:193:LEU:HD13 | 1:B:200:PHE:CE2  | 2.49                     | 0.47              |
| 1:C:90:PHE:HA    | 1:C:94:LEU:HD12  | 1.96                     | 0.47              |
| 1:C:207:GLU:O    | 1:C:210:ARG:HB3  | 2.14                     | 0.47              |
| 1:I:189:LEU:HD11 | 1:I:253:GLU:HB3  | 1.95                     | 0.47              |
| 1:J:113:LYS:HD3  | 1:J:113:LYS:N    | 2.29                     | 0.47              |
| 1:K:113:LYS:HD3  | 1:K:113:LYS:N    | 2.29                     | 0.47              |
| 1:K:260:THR:HG21 | 1:K:267:ILE:CG2  | 2.43                     | 0.47              |
| 1:A:216:LEU:HD11 | 1:A:240:TYR:HB2  | 1.95                     | 0.47              |
| 1:B:90:PHE:HA    | 1:B:94:LEU:HD12  | 1.96                     | 0.47              |
| 1:C:139:VAL:HG11 | 1:C:375:PHE:CE2  | 2.49                     | 0.47              |
| 1:J:141:SER:OG   | 1:J:339:VAL:HG22 | 2.13                     | 0.47              |
| 1:A:223:PHE:CE1  | 1:A:259:GLU:HG2  | 2.48                     | 0.47              |
| 1:C:181:ALA:O    | 1:C:185:LEU:HG   | 2.15                     | 0.47              |
| 1:D:189:LEU:HD11 | 1:D:253:GLU:HB3  | 1.95                     | 0.47              |
| 1:D:193:LEU:HD13 | 1:D:200:PHE:CE2  | 2.49                     | 0.47              |
| 1:D:290:ARG:CD   | 1:F:64:ILE:HD13  | 2.38                     | 0.47              |
| 1:E:90:PHE:HA    | 1:E:94:LEU:HD12  | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:141:SER:OG   | 1:E:339:VAL:HG22 | 2.13                     | 0.47              |
| 1:J:90:PHE:HA    | 1:J:94:LEU:HD12  | 1.96                     | 0.47              |
| 1:J:117:GLU:CA   | 1:J:367:PRO:HG2  | 2.45                     | 0.47              |
| 1:J:207:GLU:O    | 1:J:210:ARG:HB3  | 2.14                     | 0.47              |
| 1:K:189:LEU:HD11 | 1:K:253:GLU:HB3  | 1.95                     | 0.47              |
| 1:K:207:GLU:O    | 1:K:210:ARG:HB3  | 2.14                     | 0.47              |
| 1:A:113:LYS:HD3  | 1:A:113:LYS:N    | 2.29                     | 0.47              |
| 1:A:181:ALA:O    | 1:A:185:LEU:HG   | 2.15                     | 0.47              |
| 1:A:287:ILE:HB   | 1:C:64:ILE:HG22  | 1.97                     | 0.47              |
| 1:B:181:ALA:O    | 1:B:185:LEU:HG   | 2.15                     | 0.47              |
| 1:B:216:LEU:O    | 1:B:254:ARG:HG2  | 2.15                     | 0.47              |
| 1:C:113:LYS:HD3  | 1:C:113:LYS:N    | 2.29                     | 0.47              |
| 1:C:287:ILE:HB   | 1:E:64:ILE:HG22  | 1.97                     | 0.47              |
| 1:D:113:LYS:HD3  | 1:D:113:LYS:N    | 2.29                     | 0.47              |
| 1:D:216:LEU:O    | 1:D:254:ARG:HG2  | 2.15                     | 0.47              |
| 1:D:364:GLU:HG3  | 1:D:365:ALA:N    | 2.30                     | 0.47              |
| 1:E:181:ALA:O    | 1:E:185:LEU:HG   | 2.15                     | 0.47              |
| 1:F:113:LYS:N    | 1:F:113:LYS:HD3  | 2.29                     | 0.47              |
| 1:F:116:ARG:CD   | 1:F:370:VAL:HG11 | 2.43                     | 0.47              |
| 1:F:181:ALA:O    | 1:F:185:LEU:HG   | 2.15                     | 0.47              |
| 1:F:207:GLU:O    | 1:F:210:ARG:HB3  | 2.14                     | 0.47              |
| 1:G:181:ALA:O    | 1:G:185:LEU:HG   | 2.15                     | 0.47              |
| 1:H:35:VAL:O     | 1:H:67:LEU:HA    | 2.15                     | 0.47              |
| 1:H:189:LEU:HD11 | 1:H:253:GLU:HB3  | 1.95                     | 0.47              |
| 1:I:117:GLU:CA   | 1:I:367:PRO:HG2  | 2.45                     | 0.47              |
| 1:I:181:ALA:O    | 1:I:185:LEU:HG   | 2.15                     | 0.47              |
| 1:J:35:VAL:O     | 1:J:67:LEU:HA    | 2.15                     | 0.47              |
| 1:K:193:LEU:HD13 | 1:K:200:PHE:CE2  | 2.49                     | 0.47              |
| 1:A:139:VAL:HG11 | 1:A:375:PHE:CE2  | 2.49                     | 0.47              |
| 1:A:196:ARG:HH22 | 1:A:231:ALA:HA   | 1.79                     | 0.47              |
| 1:B:116:ARG:CD   | 1:B:370:VAL:HG11 | 2.43                     | 0.47              |
| 1:B:117:GLU:CA   | 1:B:367:PRO:HG2  | 2.45                     | 0.47              |
| 1:B:287:ILE:HD11 | 1:D:61:LYS:O     | 2.15                     | 0.47              |
| 1:C:117:GLU:CA   | 1:C:367:PRO:HG2  | 2.45                     | 0.47              |
| 1:D:117:GLU:CA   | 1:D:367:PRO:HG2  | 2.45                     | 0.47              |
| 1:D:181:ALA:O    | 1:D:185:LEU:HG   | 2.15                     | 0.47              |
| 1:F:35:VAL:O     | 1:F:67:LEU:HA    | 2.15                     | 0.47              |
| 1:G:117:GLU:CA   | 1:G:367:PRO:HG2  | 2.45                     | 0.47              |
| 1:G:216:LEU:HD11 | 1:G:240:TYR:HB2  | 1.95                     | 0.47              |
| 1:H:216:LEU:O    | 1:H:254:ARG:HG2  | 2.15                     | 0.47              |
| 1:K:181:ALA:O    | 1:K:185:LEU:HG   | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:117:GLU:CA   | 1:A:367:PRO:HG2  | 2.45                     | 0.47              |
| 1:D:35:VAL:O     | 1:D:67:LEU:HA    | 2.15                     | 0.47              |
| 1:D:116:ARG:CD   | 1:D:370:VAL:HG11 | 2.43                     | 0.47              |
| 1:F:189:LEU:HD11 | 1:F:253:GLU:HB3  | 1.95                     | 0.47              |
| 1:H:216:LEU:HD11 | 1:H:240:TYR:HB2  | 1.95                     | 0.47              |
| 1:I:113:LYS:N    | 1:I:113:LYS:HD3  | 2.29                     | 0.47              |
| 1:I:287:ILE:HD11 | 1:K:61:LYS:O     | 2.15                     | 0.47              |
| 1:A:190:MET:HG2  | 1:A:209:VAL:HG21 | 1.97                     | 0.47              |
| 1:C:216:LEU:O    | 1:C:254:ARG:HG2  | 2.15                     | 0.47              |
| 1:D:287:ILE:HD11 | 1:F:61:LYS:O     | 2.15                     | 0.47              |
| 1:F:216:LEU:O    | 1:F:254:ARG:HG2  | 2.15                     | 0.47              |
| 1:G:38:PRO:HG3   | 1:G:44:MET:HG2   | 1.97                     | 0.47              |
| 1:G:216:LEU:O    | 1:G:254:ARG:HG2  | 2.15                     | 0.47              |
| 1:H:181:ALA:O    | 1:H:185:LEU:HG   | 2.15                     | 0.47              |
| 1:H:221:LEU:O    | 1:H:315:LYS:HG2  | 2.15                     | 0.47              |
| 1:J:181:ALA:O    | 1:J:185:LEU:HG   | 2.15                     | 0.47              |
| 1:K:38:PRO:HG3   | 1:K:44:MET:HG2   | 1.97                     | 0.47              |
| 1:A:35:VAL:O     | 1:A:67:LEU:HA    | 2.15                     | 0.46              |
| 1:B:35:VAL:O     | 1:B:67:LEU:HA    | 2.15                     | 0.46              |
| 1:D:196:ARG:HH22 | 1:D:231:ALA:HA   | 1.79                     | 0.46              |
| 1:E:287:ILE:HD11 | 1:G:61:LYS:O     | 2.15                     | 0.46              |
| 1:G:207:GLU:O    | 1:G:210:ARG:HB3  | 2.14                     | 0.46              |
| 1:H:117:GLU:CA   | 1:H:367:PRO:HG2  | 2.45                     | 0.46              |
| 1:I:364:GLU:HG3  | 1:I:365:ALA:N    | 2.30                     | 0.46              |
| 1:K:364:GLU:HG3  | 1:K:365:ALA:N    | 2.30                     | 0.46              |
| 1:E:169:TYR:HD2  | 1:E:375:PHE:HA   | 1.81                     | 0.46              |
| 1:F:38:PRO:HG3   | 1:F:44:MET:HG2   | 1.98                     | 0.46              |
| 1:G:169:TYR:HD2  | 1:G:375:PHE:HA   | 1.81                     | 0.46              |
| 1:H:364:GLU:HG3  | 1:H:365:ALA:N    | 2.30                     | 0.46              |
| 1:J:189:LEU:HD11 | 1:J:253:GLU:HB3  | 1.95                     | 0.46              |
| 1:J:190:MET:HG2  | 1:J:209:VAL:HG21 | 1.97                     | 0.46              |
| 1:A:221:LEU:O    | 1:A:315:LYS:HG2  | 2.15                     | 0.46              |
| 1:A:290:ARG:CD   | 1:C:64:ILE:HD13  | 2.38                     | 0.46              |
| 1:C:35:VAL:O     | 1:C:67:LEU:HA    | 2.15                     | 0.46              |
| 1:F:196:ARG:HH22 | 1:F:231:ALA:HA   | 1.79                     | 0.46              |
| 1:H:90:PHE:HA    | 1:H:94:LEU:HD12  | 1.96                     | 0.46              |
| 1:H:190:MET:HG2  | 1:H:209:VAL:HG21 | 1.97                     | 0.46              |
| 1:H:207:GLU:O    | 1:H:210:ARG:HB3  | 2.14                     | 0.46              |
| 1:H:287:ILE:HD11 | 1:J:61:LYS:O     | 2.15                     | 0.46              |
| 1:I:216:LEU:O    | 1:I:254:ARG:HG2  | 2.15                     | 0.46              |
| 1:J:221:LEU:O    | 1:J:315:LYS:HG2  | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:221:LEU:O    | 1:K:315:LYS:HG2  | 2.15                     | 0.46              |
| 1:A:286:ASP:O    | 1:A:289:ILE:HG12 | 2.16                     | 0.46              |
| 1:A:287:ILE:HD11 | 1:C:61:LYS:O     | 2.15                     | 0.46              |
| 1:B:286:ASP:O    | 1:B:289:ILE:HG12 | 2.16                     | 0.46              |
| 1:D:38:PRO:HG3   | 1:D:44:MET:HG2   | 1.98                     | 0.46              |
| 1:E:190:MET:HG2  | 1:E:209:VAL:HG21 | 1.97                     | 0.46              |
| 1:E:216:LEU:O    | 1:E:254:ARG:HG2  | 2.15                     | 0.46              |
| 1:F:221:LEU:O    | 1:F:315:LYS:HG2  | 2.15                     | 0.46              |
| 1:H:263:GLN:O    | 1:H:266:PHE:HD1  | 1.99                     | 0.46              |
| 1:I:90:PHE:HA    | 1:I:94:LEU:HD12  | 1.96                     | 0.46              |
| 1:J:38:PRO:HG3   | 1:J:44:MET:HG2   | 1.97                     | 0.46              |
| 1:A:207:GLU:O    | 1:A:210:ARG:HB3  | 2.14                     | 0.46              |
| 1:F:117:GLU:CA   | 1:F:367:PRO:HG2  | 2.45                     | 0.46              |
| 1:G:364:GLU:HG3  | 1:G:365:ALA:N    | 2.30                     | 0.46              |
| 1:I:221:LEU:O    | 1:I:315:LYS:HG2  | 2.15                     | 0.46              |
| 1:K:35:VAL:O     | 1:K:67:LEU:HA    | 2.15                     | 0.46              |
| 1:K:263:GLN:O    | 1:K:266:PHE:HD1  | 1.99                     | 0.46              |
| 1:B:38:PRO:HG3   | 1:B:44:MET:HG2   | 1.98                     | 0.46              |
| 1:C:190:MET:HG2  | 1:C:209:VAL:HG21 | 1.97                     | 0.46              |
| 1:C:287:ILE:HD11 | 1:E:61:LYS:O     | 2.15                     | 0.46              |
| 1:E:173:HIS:CE1  | 1:G:45:VAL:CG1   | 2.85                     | 0.46              |
| 1:E:286:ASP:O    | 1:E:289:ILE:HG12 | 2.16                     | 0.46              |
| 1:F:263:GLN:O    | 1:F:266:PHE:HD1  | 1.99                     | 0.46              |
| 1:G:196:ARG:HH22 | 1:G:231:ALA:HA   | 1.79                     | 0.46              |
| 1:G:286:ASP:O    | 1:G:289:ILE:HG12 | 2.16                     | 0.46              |
| 1:H:116:ARG:CD   | 1:H:370:VAL:HG11 | 2.43                     | 0.46              |
| 1:K:39:ARG:HG2   | 1:K:64:ILE:O     | 2.16                     | 0.46              |
| 1:K:196:ARG:HH22 | 1:K:231:ALA:HA   | 1.79                     | 0.46              |
| 1:A:38:PRO:HG3   | 1:A:44:MET:HG2   | 1.97                     | 0.46              |
| 1:A:116:ARG:CD   | 1:A:370:VAL:HG11 | 2.43                     | 0.46              |
| 1:C:39:ARG:HG2   | 1:C:64:ILE:O     | 2.16                     | 0.46              |
| 1:D:286:ASP:O    | 1:D:289:ILE:HG12 | 2.16                     | 0.46              |
| 1:E:35:VAL:O     | 1:E:67:LEU:HA    | 2.15                     | 0.46              |
| 1:I:263:GLN:O    | 1:I:266:PHE:HD1  | 1.99                     | 0.46              |
| 1:J:116:ARG:CD   | 1:J:370:VAL:HG11 | 2.43                     | 0.46              |
| 1:J:286:ASP:O    | 1:J:289:ILE:HG12 | 2.16                     | 0.46              |
| 1:K:117:GLU:CA   | 1:K:367:PRO:HG2  | 2.45                     | 0.46              |
| 1:K:216:LEU:O    | 1:K:254:ARG:HG2  | 2.15                     | 0.46              |
| 1:K:286:ASP:O    | 1:K:289:ILE:HG12 | 2.16                     | 0.46              |
| 1:B:39:ARG:HG2   | 1:B:64:ILE:O     | 2.16                     | 0.46              |
| 1:C:263:GLN:O    | 1:C:266:PHE:HD1  | 1.99                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:38:PRO:HG3   | 1:E:44:MET:HG2   | 1.97                     | 0.46              |
| 1:E:39:ARG:HG2   | 1:E:64:ILE:O     | 2.16                     | 0.46              |
| 1:E:117:GLU:CA   | 1:E:367:PRO:HG2  | 2.45                     | 0.46              |
| 1:F:287:ILE:HD11 | 1:H:61:LYS:O     | 2.15                     | 0.46              |
| 1:F:364:GLU:HG3  | 1:F:365:ALA:N    | 2.30                     | 0.46              |
| 1:G:39:ARG:HG2   | 1:G:64:ILE:O     | 2.16                     | 0.46              |
| 1:G:139:VAL:HA   | 1:G:165:ILE:HD13 | 1.98                     | 0.46              |
| 1:A:39:ARG:HG2   | 1:A:64:ILE:O     | 2.16                     | 0.46              |
| 1:B:263:GLN:O    | 1:B:266:PHE:HD1  | 1.99                     | 0.46              |
| 1:E:263:GLN:O    | 1:E:266:PHE:HD1  | 1.99                     | 0.46              |
| 1:F:39:ARG:HG2   | 1:F:64:ILE:O     | 2.16                     | 0.46              |
| 1:F:250:ILE:CG1  | 1:F:253:GLU:HB2  | 2.46                     | 0.46              |
| 1:G:221:LEU:O    | 1:G:315:LYS:HG2  | 2.15                     | 0.46              |
| 1:H:287:ILE:HB   | 1:J:64:ILE:HG22  | 1.97                     | 0.46              |
| 1:J:216:LEU:O    | 1:J:254:ARG:HG2  | 2.15                     | 0.46              |
| 1:A:364:GLU:HG3  | 1:A:365:ALA:N    | 2.30                     | 0.46              |
| 1:B:196:ARG:HH22 | 1:B:231:ALA:HA   | 1.79                     | 0.46              |
| 1:C:169:TYR:HD2  | 1:C:375:PHE:HA   | 1.80                     | 0.46              |
| 1:C:286:ASP:O    | 1:C:289:ILE:HG12 | 2.16                     | 0.46              |
| 1:E:139:VAL:HA   | 1:E:165:ILE:HD13 | 1.98                     | 0.46              |
| 1:E:208:ILE:HG21 | 1:E:248:ILE:HG21 | 1.98                     | 0.46              |
| 1:E:364:GLU:HG3  | 1:E:365:ALA:N    | 2.30                     | 0.46              |
| 1:G:35:VAL:O     | 1:G:67:LEU:HA    | 2.15                     | 0.46              |
| 1:H:169:TYR:HD2  | 1:H:375:PHE:HA   | 1.80                     | 0.46              |
| 1:H:286:ASP:O    | 1:H:289:ILE:HG12 | 2.16                     | 0.46              |
| 1:I:250:ILE:CG1  | 1:I:253:GLU:HB2  | 2.46                     | 0.46              |
| 1:J:364:GLU:HG3  | 1:J:365:ALA:N    | 2.30                     | 0.46              |
| 1:A:263:GLN:O    | 1:A:266:PHE:HD1  | 1.99                     | 0.45              |
| 1:B:364:GLU:HG3  | 1:B:365:ALA:N    | 2.30                     | 0.45              |
| 1:C:116:ARG:CD   | 1:C:370:VAL:HG11 | 2.43                     | 0.45              |
| 1:E:152:VAL:HA   | 1:E:298:VAL:O    | 2.16                     | 0.45              |
| 1:F:190:MET:HG2  | 1:F:209:VAL:HG21 | 1.97                     | 0.45              |
| 1:F:287:ILE:HB   | 1:H:64:ILE:HG22  | 1.97                     | 0.45              |
| 1:G:190:MET:HG2  | 1:G:209:VAL:HG21 | 1.97                     | 0.45              |
| 1:I:208:ILE:HG21 | 1:I:248:ILE:HG21 | 1.98                     | 0.45              |
| 1:J:250:ILE:CG1  | 1:J:253:GLU:HB2  | 2.46                     | 0.45              |
| 1:B:221:LEU:O    | 1:B:315:LYS:HG2  | 2.15                     | 0.45              |
| 1:D:287:ILE:HB   | 1:F:64:ILE:HG22  | 1.97                     | 0.45              |
| 1:E:31:PHE:HZ    | 1:E:89:THR:HG1   | 1.65                     | 0.45              |
| 1:E:250:ILE:CG1  | 1:E:253:GLU:HB2  | 2.46                     | 0.45              |
| 1:G:263:GLN:O    | 1:G:266:PHE:HD1  | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:312:ARG:HH12 | 1:G:316:GLU:HG3  | 1.82                     | 0.45              |
| 1:H:39:ARG:HG2   | 1:H:64:ILE:O     | 2.16                     | 0.45              |
| 1:I:39:ARG:HG2   | 1:I:64:ILE:O     | 2.16                     | 0.45              |
| 1:I:190:MET:HG2  | 1:I:209:VAL:HG21 | 1.97                     | 0.45              |
| 1:J:263:GLN:O    | 1:J:266:PHE:HD1  | 1.99                     | 0.45              |
| 1:B:152:VAL:HA   | 1:B:298:VAL:O    | 2.17                     | 0.45              |
| 1:B:189:LEU:HB2  | 1:B:257:CYS:SG   | 2.57                     | 0.45              |
| 1:C:38:PRO:HG3   | 1:C:44:MET:HG2   | 1.97                     | 0.45              |
| 1:C:152:VAL:HA   | 1:C:298:VAL:O    | 2.17                     | 0.45              |
| 1:C:208:ILE:HG21 | 1:C:248:ILE:HG21 | 1.98                     | 0.45              |
| 1:D:31:PHE:CE2   | 1:D:93:GLU:HG3   | 2.52                     | 0.45              |
| 1:D:221:LEU:O    | 1:D:315:LYS:HG2  | 2.15                     | 0.45              |
| 1:D:250:ILE:CG1  | 1:D:253:GLU:HB2  | 2.46                     | 0.45              |
| 1:E:116:ARG:CD   | 1:E:370:VAL:HG11 | 2.43                     | 0.45              |
| 1:F:189:LEU:HB2  | 1:F:257:CYS:SG   | 2.57                     | 0.45              |
| 1:G:287:ILE:HD11 | 1:I:61:LYS:O     | 2.15                     | 0.45              |
| 1:K:250:ILE:CG1  | 1:K:253:GLU:HB2  | 2.46                     | 0.45              |
| 1:A:70:PRO:HG3   | 1:A:85:ILE:HD12  | 1.99                     | 0.45              |
| 1:A:216:LEU:O    | 1:A:254:ARG:HG2  | 2.15                     | 0.45              |
| 1:B:31:PHE:CE2   | 1:B:93:GLU:HG3   | 2.52                     | 0.45              |
| 1:C:221:LEU:O    | 1:C:315:LYS:HG2  | 2.15                     | 0.45              |
| 1:D:190:MET:HG2  | 1:D:209:VAL:HG21 | 1.97                     | 0.45              |
| 1:E:312:ARG:HH12 | 1:E:316:GLU:HG3  | 1.82                     | 0.45              |
| 1:F:169:TYR:HD2  | 1:F:375:PHE:HA   | 1.81                     | 0.45              |
| 1:G:208:ILE:HG21 | 1:G:248:ILE:HG21 | 1.98                     | 0.45              |
| 1:G:366:GLY:O    | 1:G:369:ILE:HG22 | 2.17                     | 0.45              |
| 1:H:38:PRO:HG3   | 1:H:44:MET:HG2   | 1.97                     | 0.45              |
| 1:I:38:PRO:HG3   | 1:I:44:MET:HG2   | 1.97                     | 0.45              |
| 1:J:152:VAL:HA   | 1:J:298:VAL:O    | 2.17                     | 0.45              |
| 1:K:70:PRO:HG3   | 1:K:85:ILE:HD12  | 1.99                     | 0.45              |
| 1:K:142:LEU:HD22 | 1:K:165:ILE:HB   | 1.98                     | 0.45              |
| 1:K:208:ILE:HG21 | 1:K:248:ILE:HG21 | 1.98                     | 0.45              |
| 1:K:289:ILE:O    | 1:K:293:LEU:HG   | 2.17                     | 0.45              |
| 1:A:173:HIS:CE1  | 1:C:45:VAL:CG1   | 2.85                     | 0.45              |
| 1:A:250:ILE:CG1  | 1:A:253:GLU:HB2  | 2.46                     | 0.45              |
| 1:A:312:ARG:NH1  | 1:A:316:GLU:HG2  | 2.32                     | 0.45              |
| 1:B:139:VAL:HA   | 1:B:165:ILE:HD13 | 1.98                     | 0.45              |
| 1:D:152:VAL:HA   | 1:D:298:VAL:O    | 2.17                     | 0.45              |
| 1:D:366:GLY:O    | 1:D:369:ILE:HG22 | 2.17                     | 0.45              |
| 1:F:286:ASP:O    | 1:F:289:ILE:HG12 | 2.16                     | 0.45              |
| 1:F:312:ARG:NH1  | 1:F:316:GLU:HG2  | 2.32                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:152:VAL:HA   | 1:G:298:VAL:O    | 2.17                     | 0.45              |
| 1:H:31:PHE:CE2   | 1:H:93:GLU:HG3   | 2.52                     | 0.45              |
| 1:H:152:VAL:HA   | 1:H:298:VAL:O    | 2.16                     | 0.45              |
| 1:I:139:VAL:HA   | 1:I:165:ILE:HD13 | 1.98                     | 0.45              |
| 1:I:286:ASP:O    | 1:I:289:ILE:HG12 | 2.16                     | 0.45              |
| 1:K:366:GLY:O    | 1:K:369:ILE:HG22 | 2.17                     | 0.45              |
| 1:B:242:LEU:CG   | 1:B:243:PRO:HD2  | 2.47                     | 0.45              |
| 1:B:287:ILE:HB   | 1:D:64:ILE:HG22  | 1.97                     | 0.45              |
| 1:D:242:LEU:CG   | 1:D:243:PRO:HD2  | 2.47                     | 0.45              |
| 1:D:289:ILE:O    | 1:D:293:LEU:HG   | 2.17                     | 0.45              |
| 1:F:31:PHE:CE2   | 1:F:93:GLU:HG3   | 2.52                     | 0.45              |
| 1:F:242:LEU:CG   | 1:F:243:PRO:HD2  | 2.47                     | 0.45              |
| 1:G:189:LEU:HB2  | 1:G:257:CYS:SG   | 2.57                     | 0.45              |
| 1:H:70:PRO:HG3   | 1:H:85:ILE:HD12  | 1.99                     | 0.45              |
| 1:I:312:ARG:HH12 | 1:I:316:GLU:HG3  | 1.82                     | 0.45              |
| 1:J:39:ARG:HG2   | 1:J:64:ILE:O     | 2.16                     | 0.45              |
| 1:J:189:LEU:HB2  | 1:J:257:CYS:SG   | 2.57                     | 0.45              |
| 1:J:312:ARG:NH1  | 1:J:316:GLU:HG2  | 2.32                     | 0.45              |
| 1:A:189:LEU:HB2  | 1:A:257:CYS:SG   | 2.57                     | 0.45              |
| 1:A:208:ILE:HG21 | 1:A:248:ILE:HG21 | 1.98                     | 0.45              |
| 1:B:142:LEU:HD22 | 1:B:165:ILE:HB   | 1.98                     | 0.45              |
| 1:B:312:ARG:NH1  | 1:B:316:GLU:HG2  | 2.32                     | 0.45              |
| 1:C:70:PRO:HG3   | 1:C:85:ILE:HD12  | 1.99                     | 0.45              |
| 1:D:263:GLN:O    | 1:D:266:PHE:HD1  | 1.99                     | 0.45              |
| 1:E:70:PRO:HG3   | 1:E:85:ILE:HD12  | 1.99                     | 0.45              |
| 1:E:221:LEU:O    | 1:E:315:LYS:HG2  | 2.15                     | 0.45              |
| 1:F:312:ARG:HH12 | 1:F:316:GLU:HG3  | 1.82                     | 0.45              |
| 1:G:116:ARG:CD   | 1:G:370:VAL:HG11 | 2.43                     | 0.45              |
| 1:H:196:ARG:HH22 | 1:H:231:ALA:HA   | 1.79                     | 0.45              |
| 1:H:312:ARG:HH12 | 1:H:316:GLU:HG3  | 1.82                     | 0.45              |
| 1:I:31:PHE:CE2   | 1:I:93:GLU:HG3   | 2.52                     | 0.45              |
| 1:I:70:PRO:HG3   | 1:I:85:ILE:HD12  | 1.99                     | 0.45              |
| 1:I:242:LEU:CG   | 1:I:243:PRO:HD2  | 2.47                     | 0.45              |
| 1:J:196:ARG:HH22 | 1:J:231:ALA:HA   | 1.79                     | 0.45              |
| 1:J:366:GLY:O    | 1:J:369:ILE:HG22 | 2.17                     | 0.45              |
| 1:A:139:VAL:HA   | 1:A:165:ILE:HD13 | 1.98                     | 0.45              |
| 1:B:250:ILE:CG1  | 1:B:253:GLU:HB2  | 2.46                     | 0.45              |
| 1:C:364:GLU:HG3  | 1:C:365:ALA:N    | 2.30                     | 0.45              |
| 1:F:70:PRO:HG3   | 1:F:85:ILE:HD12  | 1.99                     | 0.45              |
| 1:G:70:PRO:HG3   | 1:G:85:ILE:HD12  | 1.99                     | 0.45              |
| 1:H:287:ILE:CA   | 1:J:64:ILE:HG21  | 2.47                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:35:VAL:O     | 1:I:67:LEU:HA    | 2.15                     | 0.45              |
| 1:I:142:LEU:HD22 | 1:I:165:ILE:HB   | 1.98                     | 0.45              |
| 1:I:287:ILE:CA   | 1:K:64:ILE:HG21  | 2.47                     | 0.45              |
| 1:I:366:GLY:O    | 1:I:369:ILE:HG22 | 2.17                     | 0.45              |
| 1:J:139:VAL:HA   | 1:J:165:ILE:HD13 | 1.98                     | 0.45              |
| 1:J:142:LEU:HD22 | 1:J:165:ILE:HB   | 1.98                     | 0.45              |
| 1:K:116:ARG:CD   | 1:K:370:VAL:HG11 | 2.43                     | 0.45              |
| 1:K:189:LEU:HB2  | 1:K:257:CYS:SG   | 2.57                     | 0.45              |
| 1:K:190:MET:HG2  | 1:K:209:VAL:HG21 | 1.97                     | 0.45              |
| 1:K:242:LEU:CG   | 1:K:243:PRO:HD2  | 2.47                     | 0.45              |
| 1:A:142:LEU:HD22 | 1:A:165:ILE:HB   | 1.98                     | 0.45              |
| 1:A:152:VAL:HA   | 1:A:298:VAL:O    | 2.17                     | 0.45              |
| 1:B:289:ILE:O    | 1:B:293:LEU:HG   | 2.17                     | 0.45              |
| 1:B:312:ARG:HH12 | 1:B:316:GLU:HG3  | 1.82                     | 0.45              |
| 1:C:250:ILE:CG1  | 1:C:253:GLU:HB2  | 2.46                     | 0.45              |
| 1:C:312:ARG:HH12 | 1:C:316:GLU:HG3  | 1.82                     | 0.45              |
| 1:D:312:ARG:HH12 | 1:D:316:GLU:HG3  | 1.82                     | 0.45              |
| 1:E:366:GLY:O    | 1:E:369:ILE:HG22 | 2.17                     | 0.45              |
| 1:H:139:VAL:HA   | 1:H:165:ILE:HD13 | 1.98                     | 0.45              |
| 1:H:189:LEU:HB2  | 1:H:257:CYS:SG   | 2.57                     | 0.45              |
| 1:H:242:LEU:CG   | 1:H:243:PRO:HD2  | 2.47                     | 0.45              |
| 1:H:250:ILE:CG1  | 1:H:253:GLU:HB2  | 2.46                     | 0.45              |
| 1:H:366:GLY:O    | 1:H:369:ILE:HG22 | 2.17                     | 0.45              |
| 1:I:152:VAL:HA   | 1:I:298:VAL:O    | 2.16                     | 0.45              |
| 1:I:189:LEU:HB2  | 1:I:257:CYS:SG   | 2.57                     | 0.45              |
| 1:K:31:PHE:CE2   | 1:K:93:GLU:HG3   | 2.52                     | 0.45              |
| 1:A:242:LEU:CG   | 1:A:243:PRO:HD2  | 2.47                     | 0.45              |
| 1:B:190:MET:HG2  | 1:B:209:VAL:HG21 | 1.97                     | 0.45              |
| 1:B:371:HIS:CE1  | 1:C:201:VAL:HG11 | 2.52                     | 0.45              |
| 1:C:366:GLY:O    | 1:C:369:ILE:HG22 | 2.17                     | 0.45              |
| 1:D:371:HIS:CE1  | 1:E:201:VAL:HG11 | 2.53                     | 0.45              |
| 1:F:152:VAL:HA   | 1:F:298:VAL:O    | 2.17                     | 0.45              |
| 1:F:287:ILE:CA   | 1:H:64:ILE:HG21  | 2.47                     | 0.45              |
| 1:I:312:ARG:NH1  | 1:I:316:GLU:HG2  | 2.32                     | 0.45              |
| 1:J:70:PRO:HG3   | 1:J:85:ILE:HD12  | 1.99                     | 0.45              |
| 1:K:312:ARG:NH1  | 1:K:316:GLU:HG2  | 2.32                     | 0.45              |
| 1:B:70:PRO:HG3   | 1:B:85:ILE:HD12  | 1.99                     | 0.44              |
| 1:B:287:ILE:HG21 | 1:D:65:LEU:HG    | 1.99                     | 0.44              |
| 1:D:39:ARG:HG2   | 1:D:64:ILE:O     | 2.16                     | 0.44              |
| 1:D:208:ILE:HG21 | 1:D:248:ILE:HG21 | 1.98                     | 0.44              |
| 1:D:312:ARG:NH1  | 1:D:316:GLU:HG2  | 2.32                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:289:ILE:O    | 1:F:293:LEU:HG   | 2.17                     | 0.44              |
| 1:F:366:GLY:O    | 1:F:369:ILE:HG22 | 2.17                     | 0.44              |
| 1:F:371:HIS:CE1  | 1:G:201:VAL:HG11 | 2.53                     | 0.44              |
| 1:G:287:ILE:CA   | 1:I:64:ILE:HG21  | 2.47                     | 0.44              |
| 1:H:142:LEU:HD22 | 1:H:165:ILE:HB   | 1.98                     | 0.44              |
| 1:H:208:ILE:HG21 | 1:H:248:ILE:HG21 | 1.98                     | 0.44              |
| 1:J:31:PHE:CE2   | 1:J:93:GLU:HG3   | 2.52                     | 0.44              |
| 1:J:289:ILE:O    | 1:J:293:LEU:HG   | 2.17                     | 0.44              |
| 1:A:56:ASP:HA    | 1:A:59:GLN:CD    | 2.43                     | 0.44              |
| 1:A:366:GLY:O    | 1:A:369:ILE:HG22 | 2.17                     | 0.44              |
| 1:D:56:ASP:HA    | 1:D:59:GLN:CD    | 2.43                     | 0.44              |
| 1:E:189:LEU:HB2  | 1:E:257:CYS:SG   | 2.57                     | 0.44              |
| 1:E:286:ASP:OD2  | 1:G:47:MET:SD    | 2.76                     | 0.44              |
| 1:E:287:ILE:CA   | 1:G:64:ILE:HG21  | 2.47                     | 0.44              |
| 1:F:139:VAL:HA   | 1:F:165:ILE:HD13 | 1.98                     | 0.44              |
| 1:G:21:PHE:HB2   | 1:G:24:ASP:OD1   | 2.17                     | 0.44              |
| 1:G:31:PHE:CE2   | 1:G:93:GLU:HG3   | 2.52                     | 0.44              |
| 1:H:287:ILE:HG21 | 1:J:65:LEU:HG    | 1.99                     | 0.44              |
| 1:I:116:ARG:CD   | 1:I:370:VAL:HG11 | 2.43                     | 0.44              |
| 1:I:286:ASP:OD2  | 1:K:47:MET:SD    | 2.76                     | 0.44              |
| 1:J:312:ARG:HH12 | 1:J:316:GLU:HG3  | 1.82                     | 0.44              |
| 1:K:21:PHE:HB2   | 1:K:24:ASP:OD1   | 2.17                     | 0.44              |
| 1:K:31:PHE:HZ    | 1:K:89:THR:HG1   | 1.65                     | 0.44              |
| 1:K:169:TYR:HD2  | 1:K:375:PHE:HA   | 1.80                     | 0.44              |
| 1:K:312:ARG:HH12 | 1:K:316:GLU:HG3  | 1.82                     | 0.44              |
| 1:A:287:ILE:CA   | 1:C:64:ILE:HG21  | 2.47                     | 0.44              |
| 1:B:287:ILE:CA   | 1:D:64:ILE:HG21  | 2.47                     | 0.44              |
| 1:C:142:LEU:HD22 | 1:C:165:ILE:HB   | 1.99                     | 0.44              |
| 1:C:189:LEU:HB2  | 1:C:257:CYS:SG   | 2.57                     | 0.44              |
| 1:C:286:ASP:OD2  | 1:E:47:MET:SD    | 2.76                     | 0.44              |
| 1:D:142:LEU:HD22 | 1:D:165:ILE:HB   | 1.98                     | 0.44              |
| 1:E:312:ARG:NH1  | 1:E:316:GLU:HG2  | 2.32                     | 0.44              |
| 1:F:56:ASP:HA    | 1:F:59:GLN:CD    | 2.43                     | 0.44              |
| 1:F:286:ASP:OD2  | 1:H:47:MET:SD    | 2.76                     | 0.44              |
| 1:G:242:LEU:CG   | 1:G:243:PRO:HD2  | 2.47                     | 0.44              |
| 1:G:250:ILE:CG1  | 1:G:253:GLU:HB2  | 2.46                     | 0.44              |
| 1:G:286:ASP:OD2  | 1:I:47:MET:SD    | 2.76                     | 0.44              |
| 1:H:312:ARG:NH1  | 1:H:316:GLU:HG2  | 2.32                     | 0.44              |
| 1:H:371:HIS:CE1  | 1:I:201:VAL:HG11 | 2.52                     | 0.44              |
| 1:J:242:LEU:CG   | 1:J:243:PRO:HD2  | 2.47                     | 0.44              |
| 1:K:152:VAL:HA   | 1:K:298:VAL:O    | 2.16                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:31:PHE:CE2   | 1:A:93:GLU:HG3   | 2.52                     | 0.44              |
| 1:B:56:ASP:HA    | 1:B:59:GLN:CD    | 2.43                     | 0.44              |
| 1:B:155:SER:HB3  | 1:B:304:THR:HG23 | 2.00                     | 0.44              |
| 1:C:312:ARG:NH1  | 1:C:316:GLU:HG2  | 2.32                     | 0.44              |
| 1:D:242:LEU:HG   | 1:D:243:PRO:HD2  | 2.00                     | 0.44              |
| 1:D:287:ILE:CA   | 1:F:64:ILE:HG21  | 2.47                     | 0.44              |
| 1:E:289:ILE:O    | 1:E:293:LEU:HG   | 2.17                     | 0.44              |
| 1:F:208:ILE:HG21 | 1:F:248:ILE:HG21 | 1.98                     | 0.44              |
| 1:F:290:ARG:O    | 1:F:294:TYR:HD2  | 2.01                     | 0.44              |
| 1:G:275:HIS:HB2  | 1:G:317:ILE:CD1  | 2.48                     | 0.44              |
| 1:G:289:ILE:O    | 1:G:293:LEU:HG   | 2.17                     | 0.44              |
| 1:H:56:ASP:HA    | 1:H:59:GLN:CD    | 2.43                     | 0.44              |
| 1:I:196:ARG:HH22 | 1:I:231:ALA:HA   | 1.79                     | 0.44              |
| 1:J:208:ILE:HG21 | 1:J:248:ILE:HG21 | 1.98                     | 0.44              |
| 1:K:56:ASP:HA    | 1:K:59:GLN:CD    | 2.43                     | 0.44              |
| 1:B:208:ILE:HG21 | 1:B:248:ILE:HG21 | 1.98                     | 0.44              |
| 1:B:286:ASP:OD2  | 1:D:47:MET:SD    | 2.76                     | 0.44              |
| 1:B:366:GLY:O    | 1:B:369:ILE:HG22 | 2.17                     | 0.44              |
| 1:C:155:SER:HB3  | 1:C:304:THR:HG23 | 2.00                     | 0.44              |
| 1:C:287:ILE:CA   | 1:E:64:ILE:HG21  | 2.47                     | 0.44              |
| 1:E:56:ASP:HA    | 1:E:59:GLN:CD    | 2.43                     | 0.44              |
| 1:F:275:HIS:HB2  | 1:F:317:ILE:CD1  | 2.48                     | 0.44              |
| 1:G:371:HIS:CE1  | 1:H:201:VAL:HG11 | 2.52                     | 0.44              |
| 1:H:286:ASP:OD2  | 1:J:47:MET:SD    | 2.76                     | 0.44              |
| 1:I:289:ILE:O    | 1:I:293:LEU:HG   | 2.17                     | 0.44              |
| 1:K:139:VAL:HA   | 1:K:165:ILE:HD13 | 1.98                     | 0.44              |
| 1:A:71:ILE:HG12  | 1:A:76:ILE:HG12  | 2.00                     | 0.44              |
| 1:A:155:SER:HB3  | 1:A:304:THR:HG23 | 2.00                     | 0.44              |
| 1:A:286:ASP:OD2  | 1:C:47:MET:SD    | 2.76                     | 0.44              |
| 1:B:242:LEU:HG   | 1:B:243:PRO:HD2  | 2.00                     | 0.44              |
| 1:C:242:LEU:CG   | 1:C:243:PRO:HD2  | 2.47                     | 0.44              |
| 1:C:275:HIS:HB2  | 1:C:317:ILE:CD1  | 2.48                     | 0.44              |
| 1:C:289:ILE:O    | 1:C:293:LEU:HG   | 2.17                     | 0.44              |
| 1:D:139:VAL:HA   | 1:D:165:ILE:HD13 | 1.98                     | 0.44              |
| 1:D:169:TYR:HD2  | 1:D:375:PHE:HA   | 1.80                     | 0.44              |
| 1:F:166:TYR:HB2  | 1:F:289:ILE:HD13 | 2.00                     | 0.44              |
| 1:G:142:LEU:HD22 | 1:G:165:ILE:HB   | 1.98                     | 0.44              |
| 1:G:312:ARG:NH1  | 1:G:316:GLU:HG2  | 2.32                     | 0.44              |
| 1:H:287:ILE:HD12 | 1:J:64:ILE:HD12  | 1.42                     | 0.44              |
| 1:H:290:ARG:O    | 1:H:294:TYR:HD2  | 2.01                     | 0.44              |
| 1:I:371:HIS:CE1  | 1:J:201:VAL:HG11 | 2.53                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:71:ILE:HG12  | 1:J:76:ILE:HG12  | 2.00                     | 0.44              |
| 1:A:275:HIS:HB2  | 1:A:317:ILE:CD1  | 2.48                     | 0.44              |
| 1:B:275:HIS:HB2  | 1:B:317:ILE:CD1  | 2.48                     | 0.44              |
| 1:C:31:PHE:CE2   | 1:C:93:GLU:HG3   | 2.52                     | 0.44              |
| 1:C:71:ILE:HG12  | 1:C:76:ILE:HG12  | 2.00                     | 0.44              |
| 1:C:139:VAL:HA   | 1:C:165:ILE:HD13 | 1.98                     | 0.44              |
| 1:D:189:LEU:HB2  | 1:D:257:CYS:SG   | 2.57                     | 0.44              |
| 1:D:286:ASP:OD2  | 1:F:47:MET:SD    | 2.76                     | 0.44              |
| 1:D:290:ARG:O    | 1:D:294:TYR:HD2  | 2.01                     | 0.44              |
| 1:E:142:LEU:HD22 | 1:E:165:ILE:HB   | 1.99                     | 0.44              |
| 1:E:371:HIS:CE1  | 1:F:201:VAL:HG11 | 2.52                     | 0.44              |
| 1:F:142:LEU:HD22 | 1:F:165:ILE:HB   | 1.99                     | 0.44              |
| 1:I:21:PHE:HB2   | 1:I:24:ASP:OD1   | 2.17                     | 0.44              |
| 1:I:275:HIS:HB2  | 1:I:317:ILE:CD1  | 2.48                     | 0.44              |
| 1:I:287:ILE:HB   | 1:K:64:ILE:HG22  | 1.97                     | 0.44              |
| 1:J:371:HIS:CE1  | 1:K:201:VAL:HG11 | 2.53                     | 0.44              |
| 1:D:155:SER:HB3  | 1:D:304:THR:HG23 | 2.00                     | 0.44              |
| 1:E:155:SER:HB3  | 1:E:304:THR:HG23 | 2.00                     | 0.44              |
| 1:E:196:ARG:HH22 | 1:E:231:ALA:HA   | 1.79                     | 0.44              |
| 1:F:242:LEU:HG   | 1:F:243:PRO:HD2  | 2.00                     | 0.44              |
| 1:F:257:CYS:HB3  | 1:F:258:PRO:HD3  | 2.00                     | 0.44              |
| 1:H:289:ILE:O    | 1:H:293:LEU:HG   | 2.17                     | 0.44              |
| 1:J:275:HIS:HB2  | 1:J:317:ILE:CD1  | 2.48                     | 0.44              |
| 1:K:275:HIS:HB2  | 1:K:317:ILE:CD1  | 2.48                     | 0.44              |
| 1:A:289:ILE:O    | 1:A:293:LEU:HG   | 2.17                     | 0.44              |
| 1:C:257:CYS:HB3  | 1:C:258:PRO:HD3  | 2.00                     | 0.44              |
| 1:D:70:PRO:HG3   | 1:D:85:ILE:HD12  | 1.99                     | 0.44              |
| 1:E:31:PHE:CE2   | 1:E:93:GLU:HG3   | 2.52                     | 0.44              |
| 1:G:155:SER:HB3  | 1:G:304:THR:HG23 | 2.00                     | 0.44              |
| 1:G:257:CYS:HB3  | 1:G:258:PRO:HD3  | 2.00                     | 0.44              |
| 1:G:287:ILE:HB   | 1:I:64:ILE:HG22  | 1.97                     | 0.44              |
| 1:H:71:ILE:HG12  | 1:H:76:ILE:HG12  | 2.00                     | 0.44              |
| 1:H:275:HIS:HB2  | 1:H:317:ILE:CD1  | 2.48                     | 0.44              |
| 1:J:56:ASP:HA    | 1:J:59:GLN:CD    | 2.43                     | 0.44              |
| 1:K:242:LEU:HG   | 1:K:243:PRO:HD2  | 2.00                     | 0.44              |
| 1:A:290:ARG:O    | 1:A:294:TYR:HD2  | 2.01                     | 0.43              |
| 1:C:56:ASP:HA    | 1:C:59:GLN:CD    | 2.43                     | 0.43              |
| 1:D:166:TYR:HB2  | 1:D:289:ILE:HD13 | 2.00                     | 0.43              |
| 1:E:242:LEU:CG   | 1:E:243:PRO:HD2  | 2.47                     | 0.43              |
| 1:I:155:SER:HB3  | 1:I:304:THR:HG23 | 2.00                     | 0.43              |
| 1:I:242:LEU:HG   | 1:I:243:PRO:HD2  | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:290:ARG:O    | 1:J:294:TYR:HD2  | 2.01                     | 0.43              |
| 1:K:155:SER:HB3  | 1:K:304:THR:HG23 | 2.00                     | 0.43              |
| 1:K:290:ARG:O    | 1:K:294:TYR:HD2  | 2.01                     | 0.43              |
| 1:A:287:ILE:HG21 | 1:C:65:LEU:HG    | 1.99                     | 0.43              |
| 1:A:312:ARG:HH12 | 1:A:316:GLU:HG3  | 1.82                     | 0.43              |
| 1:A:371:HIS:CE1  | 1:B:201:VAL:HG11 | 2.52                     | 0.43              |
| 1:B:257:CYS:HB3  | 1:B:258:PRO:HD3  | 2.00                     | 0.43              |
| 1:C:21:PHE:HB2   | 1:C:24:ASP:OD1   | 2.17                     | 0.43              |
| 1:C:312:ARG:HG3  | 1:C:312:ARG:NH1  | 2.33                     | 0.43              |
| 1:C:371:HIS:CE1  | 1:D:201:VAL:HG11 | 2.53                     | 0.43              |
| 1:G:56:ASP:HA    | 1:G:59:GLN:CD    | 2.43                     | 0.43              |
| 1:H:21:PHE:HB2   | 1:H:24:ASP:OD1   | 2.17                     | 0.43              |
| 1:I:56:ASP:HA    | 1:I:59:GLN:CD    | 2.43                     | 0.43              |
| 1:I:173:HIS:CE1  | 1:K:45:VAL:CG1   | 2.85                     | 0.43              |
| 1:D:264:PRO:HD3  | 1:D:273:GLY:HA2  | 2.01                     | 0.43              |
| 1:E:71:ILE:HG12  | 1:E:76:ILE:HG12  | 2.00                     | 0.43              |
| 1:E:287:ILE:HB   | 1:G:64:ILE:HG22  | 1.97                     | 0.43              |
| 1:E:312:ARG:HG3  | 1:E:312:ARG:NH1  | 2.33                     | 0.43              |
| 1:F:155:SER:HB3  | 1:F:304:THR:HG23 | 2.00                     | 0.43              |
| 1:H:242:LEU:HG   | 1:H:243:PRO:HD2  | 2.00                     | 0.43              |
| 1:I:257:CYS:HB3  | 1:I:258:PRO:HD3  | 2.00                     | 0.43              |
| 1:A:169:TYR:HD2  | 1:A:375:PHE:HA   | 1.80                     | 0.43              |
| 1:A:257:CYS:HB3  | 1:A:258:PRO:HD3  | 2.00                     | 0.43              |
| 1:B:264:PRO:HD3  | 1:B:273:GLY:HA2  | 2.01                     | 0.43              |
| 1:B:287:ILE:HD12 | 1:D:64:ILE:HD12  | 1.42                     | 0.43              |
| 1:C:31:PHE:HZ    | 1:C:89:THR:HG1   | 1.67                     | 0.43              |
| 1:F:264:PRO:HD3  | 1:F:273:GLY:HA2  | 2.01                     | 0.43              |
| 1:G:242:LEU:HG   | 1:G:243:PRO:HD2  | 2.00                     | 0.43              |
| 1:H:257:CYS:HB3  | 1:H:258:PRO:HD3  | 2.00                     | 0.43              |
| 1:J:166:TYR:HB2  | 1:J:289:ILE:HD13 | 2.00                     | 0.43              |
| 1:B:166:TYR:HB2  | 1:B:289:ILE:HD13 | 2.00                     | 0.43              |
| 1:B:290:ARG:O    | 1:B:294:TYR:HD2  | 2.01                     | 0.43              |
| 1:C:287:ILE:HG21 | 1:E:65:LEU:HG    | 1.99                     | 0.43              |
| 1:C:290:ARG:O    | 1:C:294:TYR:HD2  | 2.01                     | 0.43              |
| 1:D:21:PHE:HB2   | 1:D:24:ASP:OD1   | 2.18                     | 0.43              |
| 1:F:71:ILE:HG12  | 1:F:76:ILE:HG12  | 2.00                     | 0.43              |
| 1:J:21:PHE:HB2   | 1:J:24:ASP:OD1   | 2.17                     | 0.43              |
| 1:J:264:PRO:HD3  | 1:J:273:GLY:HA2  | 2.01                     | 0.43              |
| 1:K:166:TYR:HB2  | 1:K:289:ILE:HD13 | 2.00                     | 0.43              |
| 1:C:166:TYR:HB2  | 1:C:289:ILE:HD13 | 2.00                     | 0.43              |
| 1:D:71:ILE:HG12  | 1:D:76:ILE:HG12  | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:21:PHE:HB2   | 1:E:24:ASP:OD1   | 2.17                     | 0.43              |
| 1:E:166:TYR:HB2  | 1:E:289:ILE:HD13 | 2.00                     | 0.43              |
| 1:H:166:TYR:HB2  | 1:H:289:ILE:HD13 | 2.00                     | 0.43              |
| 1:A:312:ARG:HG3  | 1:A:312:ARG:NH1  | 2.33                     | 0.43              |
| 1:H:155:SER:HB3  | 1:H:304:THR:HG23 | 2.00                     | 0.43              |
| 1:H:264:PRO:HD3  | 1:H:273:GLY:HA2  | 2.01                     | 0.43              |
| 1:I:290:ARG:O    | 1:I:294:TYR:HD2  | 2.01                     | 0.43              |
| 1:J:192:ILE:CG1  | 1:J:253:GLU:HG3  | 2.49                     | 0.43              |
| 1:A:21:PHE:HB2   | 1:A:24:ASP:OD1   | 2.17                     | 0.43              |
| 1:B:21:PHE:HB2   | 1:B:24:ASP:OD1   | 2.18                     | 0.43              |
| 1:D:192:ILE:CG1  | 1:D:253:GLU:HG3  | 2.49                     | 0.43              |
| 1:D:275:HIS:HB2  | 1:D:317:ILE:CD1  | 2.48                     | 0.43              |
| 1:E:113:LYS:O    | 1:E:117:GLU:HG3  | 2.19                     | 0.43              |
| 1:E:242:LEU:HG   | 1:E:243:PRO:HD2  | 2.00                     | 0.43              |
| 1:E:275:HIS:HB2  | 1:E:317:ILE:CD1  | 2.48                     | 0.43              |
| 1:F:21:PHE:HB2   | 1:F:24:ASP:OD1   | 2.17                     | 0.43              |
| 1:G:113:LYS:O    | 1:G:117:GLU:HG3  | 2.19                     | 0.43              |
| 1:G:290:ARG:O    | 1:G:294:TYR:HD2  | 2.01                     | 0.43              |
| 1:H:113:LYS:O    | 1:H:117:GLU:HG3  | 2.19                     | 0.43              |
| 1:H:192:ILE:CG1  | 1:H:253:GLU:HG3  | 2.49                     | 0.43              |
| 1:I:287:ILE:HG21 | 1:K:65:LEU:HG    | 1.99                     | 0.43              |
| 1:J:242:LEU:HG   | 1:J:243:PRO:HD2  | 2.00                     | 0.43              |
| 1:J:257:CYS:HB3  | 1:J:258:PRO:HD3  | 2.00                     | 0.43              |
| 1:B:192:ILE:CG1  | 1:B:253:GLU:HG3  | 2.49                     | 0.43              |
| 1:C:113:LYS:O    | 1:C:117:GLU:HG3  | 2.19                     | 0.43              |
| 1:D:268:GLY:HA3  | 1:E:40:HIS:CB    | 2.49                     | 0.43              |
| 1:G:287:ILE:HG21 | 1:I:65:LEU:HG    | 1.99                     | 0.43              |
| 1:H:268:GLY:HA3  | 1:I:40:HIS:CB    | 2.49                     | 0.43              |
| 1:I:113:LYS:O    | 1:I:117:GLU:HG3  | 2.19                     | 0.43              |
| 1:I:166:TYR:HB2  | 1:I:289:ILE:HD13 | 2.00                     | 0.43              |
| 1:J:113:LYS:O    | 1:J:117:GLU:HG3  | 2.19                     | 0.43              |
| 1:J:169:TYR:HD2  | 1:J:375:PHE:HA   | 1.80                     | 0.43              |
| 1:K:257:CYS:HB3  | 1:K:258:PRO:HD3  | 2.00                     | 0.43              |
| 1:B:113:LYS:O    | 1:B:117:GLU:HG3  | 2.19                     | 0.43              |
| 1:B:268:GLY:HA3  | 1:C:40:HIS:CB    | 2.49                     | 0.43              |
| 1:F:230:ALA:HB1  | 1:F:252:ASN:HB3  | 2.01                     | 0.43              |
| 1:G:71:ILE:HG12  | 1:G:76:ILE:HG12  | 2.00                     | 0.43              |
| 1:G:268:GLY:HA3  | 1:H:40:HIS:CB    | 2.49                     | 0.43              |
| 1:G:312:ARG:HG3  | 1:G:312:ARG:NH1  | 2.33                     | 0.43              |
| 1:I:169:TYR:HD2  | 1:I:375:PHE:HA   | 1.80                     | 0.43              |
| 1:J:155:SER:HB3  | 1:J:304:THR:HG23 | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:264:PRO:HD3  | 1:K:273:GLY:HA2  | 2.01                     | 0.43              |
| 1:E:290:ARG:O    | 1:E:294:TYR:HD2  | 2.01                     | 0.42              |
| 1:F:192:ILE:CG1  | 1:F:253:GLU:HG3  | 2.49                     | 0.42              |
| 1:F:268:GLY:HA3  | 1:G:40:HIS:CB    | 2.49                     | 0.42              |
| 1:G:166:TYR:HB2  | 1:G:289:ILE:HD13 | 2.00                     | 0.42              |
| 1:H:230:ALA:HB1  | 1:H:252:ASN:HB3  | 2.01                     | 0.42              |
| 1:I:268:GLY:HA3  | 1:J:40:HIS:CB    | 2.49                     | 0.42              |
| 1:J:312:ARG:HG3  | 1:J:312:ARG:NH1  | 2.33                     | 0.42              |
| 1:K:113:LYS:O    | 1:K:117:GLU:HG3  | 2.19                     | 0.42              |
| 1:A:166:TYR:HB2  | 1:A:289:ILE:HD13 | 2.00                     | 0.42              |
| 1:A:230:ALA:HB1  | 1:A:252:ASN:HB3  | 2.01                     | 0.42              |
| 1:B:71:ILE:HG12  | 1:B:76:ILE:HG12  | 2.00                     | 0.42              |
| 1:C:230:ALA:HB1  | 1:C:252:ASN:HB3  | 2.02                     | 0.42              |
| 1:D:139:VAL:HG22 | 1:D:170:ALA:HB2  | 2.02                     | 0.42              |
| 1:E:230:ALA:HB1  | 1:E:252:ASN:HB3  | 2.02                     | 0.42              |
| 1:E:257:CYS:HB3  | 1:E:258:PRO:HD3  | 2.00                     | 0.42              |
| 1:G:230:ALA:HB1  | 1:G:252:ASN:HB3  | 2.01                     | 0.42              |
| 1:J:230:ALA:HB1  | 1:J:252:ASN:HB3  | 2.02                     | 0.42              |
| 1:K:71:ILE:HG12  | 1:K:76:ILE:HG12  | 2.00                     | 0.42              |
| 1:B:353:GLN:HA   | 1:B:356:TRP:HD1  | 1.84                     | 0.42              |
| 1:G:139:VAL:HG22 | 1:G:170:ALA:HB2  | 2.02                     | 0.42              |
| 1:H:139:VAL:HG22 | 1:H:170:ALA:HB2  | 2.02                     | 0.42              |
| 1:I:71:ILE:HG12  | 1:I:76:ILE:HG12  | 2.00                     | 0.42              |
| 1:A:192:ILE:CG1  | 1:A:253:GLU:HG3  | 2.49                     | 0.42              |
| 1:B:139:VAL:HG22 | 1:B:170:ALA:HB2  | 2.02                     | 0.42              |
| 1:C:18:LYS:HG3   | 1:C:30:VAL:HG22  | 2.02                     | 0.42              |
| 1:C:192:ILE:CG1  | 1:C:253:GLU:HG3  | 2.49                     | 0.42              |
| 1:D:230:ALA:HB1  | 1:D:252:ASN:HB3  | 2.02                     | 0.42              |
| 1:G:111:ASN:HB3  | 1:G:116:ARG:HH21 | 1.85                     | 0.42              |
| 1:I:230:ALA:HB1  | 1:I:252:ASN:HB3  | 2.01                     | 0.42              |
| 1:A:113:LYS:O    | 1:A:117:GLU:HG3  | 2.19                     | 0.42              |
| 1:A:242:LEU:HG   | 1:A:243:PRO:HD2  | 2.00                     | 0.42              |
| 1:A:264:PRO:HD3  | 1:A:273:GLY:HA2  | 2.01                     | 0.42              |
| 1:A:268:GLY:HA3  | 1:B:40:HIS:CB    | 2.49                     | 0.42              |
| 1:B:111:ASN:HB3  | 1:B:116:ARG:HH21 | 1.85                     | 0.42              |
| 1:C:242:LEU:HG   | 1:C:243:PRO:HD2  | 2.00                     | 0.42              |
| 1:D:257:CYS:HB3  | 1:D:258:PRO:HD3  | 2.00                     | 0.42              |
| 1:F:287:ILE:HG21 | 1:H:65:LEU:HG    | 1.99                     | 0.42              |
| 1:I:139:VAL:HG22 | 1:I:170:ALA:HB2  | 2.02                     | 0.42              |
| 1:I:264:PRO:HD3  | 1:I:273:GLY:HA2  | 2.01                     | 0.42              |
| 1:K:139:VAL:HG22 | 1:K:170:ALA:HB2  | 2.02                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:139:VAL:HG22 | 1:A:170:ALA:HB2  | 2.01                     | 0.42              |
| 1:C:264:PRO:HD3  | 1:C:273:GLY:HA2  | 2.01                     | 0.42              |
| 1:E:139:VAL:HG22 | 1:E:170:ALA:HB2  | 2.02                     | 0.42              |
| 1:E:264:PRO:HD3  | 1:E:273:GLY:HA2  | 2.01                     | 0.42              |
| 1:F:139:VAL:HG22 | 1:F:170:ALA:HB2  | 2.02                     | 0.42              |
| 1:I:111:ASN:HB3  | 1:I:116:ARG:HH21 | 1.85                     | 0.42              |
| 1:B:169:TYR:HD2  | 1:B:375:PHE:HA   | 1.80                     | 0.42              |
| 1:B:230:ALA:HB1  | 1:B:252:ASN:HB3  | 2.02                     | 0.42              |
| 1:C:139:VAL:HG22 | 1:C:170:ALA:HB2  | 2.02                     | 0.42              |
| 1:C:268:GLY:HA3  | 1:D:40:HIS:CB    | 2.49                     | 0.42              |
| 1:E:192:ILE:CG1  | 1:E:253:GLU:HG3  | 2.49                     | 0.42              |
| 1:F:113:LYS:O    | 1:F:117:GLU:HG3  | 2.19                     | 0.42              |
| 1:F:188:TYR:CE1  | 1:F:266:PHE:HB3  | 2.55                     | 0.42              |
| 1:G:18:LYS:HG3   | 1:G:30:VAL:HG22  | 2.02                     | 0.42              |
| 1:G:264:PRO:HD3  | 1:G:273:GLY:HA2  | 2.01                     | 0.42              |
| 1:H:188:TYR:CE1  | 1:H:266:PHE:HB3  | 2.55                     | 0.42              |
| 1:H:312:ARG:HG3  | 1:H:312:ARG:NH1  | 2.33                     | 0.42              |
| 1:I:49:GLN:HG3   | 1:I:49:GLN:O     | 2.20                     | 0.42              |
| 1:K:230:ALA:HB1  | 1:K:252:ASN:HB3  | 2.01                     | 0.42              |
| 1:K:312:ARG:HG3  | 1:K:312:ARG:NH1  | 2.33                     | 0.42              |
| 1:D:353:GLN:HA   | 1:D:356:TRP:HD1  | 1.84                     | 0.42              |
| 1:I:192:ILE:CG1  | 1:I:253:GLU:HG3  | 2.49                     | 0.42              |
| 1:K:192:ILE:CG1  | 1:K:253:GLU:HG3  | 2.49                     | 0.42              |
| 1:A:49:GLN:HG3   | 1:A:49:GLN:O     | 2.20                     | 0.42              |
| 1:G:18:LYS:HD3   | 1:G:18:LYS:N     | 2.35                     | 0.42              |
| 1:G:49:GLN:HG3   | 1:G:49:GLN:O     | 2.20                     | 0.42              |
| 1:I:312:ARG:HG3  | 1:I:312:ARG:NH1  | 2.33                     | 0.42              |
| 1:J:139:VAL:HG22 | 1:J:170:ALA:HB2  | 2.02                     | 0.42              |
| 1:D:140:LEU:HD22 | 1:D:343:GLY:HA2  | 2.02                     | 0.42              |
| 1:E:111:ASN:HB3  | 1:E:116:ARG:HH21 | 1.85                     | 0.42              |
| 1:G:192:ILE:CG1  | 1:G:253:GLU:HG3  | 2.49                     | 0.42              |
| 1:J:111:ASN:HB3  | 1:J:116:ARG:HH21 | 1.85                     | 0.42              |
| 1:A:18:LYS:HG3   | 1:A:30:VAL:HG22  | 2.02                     | 0.41              |
| 1:D:111:ASN:HB3  | 1:D:116:ARG:HH21 | 1.85                     | 0.41              |
| 1:D:113:LYS:O    | 1:D:117:GLU:HG3  | 2.19                     | 0.41              |
| 1:E:268:GLY:HA3  | 1:F:40:HIS:CB    | 2.49                     | 0.41              |
| 1:F:140:LEU:HD22 | 1:F:343:GLY:HA2  | 2.02                     | 0.41              |
| 1:I:18:LYS:HD3   | 1:I:18:LYS:N     | 2.35                     | 0.41              |
| 1:J:49:GLN:O     | 1:J:49:GLN:HG3   | 2.20                     | 0.41              |
| 1:J:188:TYR:CE1  | 1:J:266:PHE:HB3  | 2.55                     | 0.41              |
| 1:J:268:GLY:HA3  | 1:K:40:HIS:CB    | 2.49                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:111:ASN:HB3  | 1:A:116:ARG:HH21 | 1.85                     | 0.41              |
| 1:D:185:LEU:HB3  | 1:D:257:CYS:SG   | 2.61                     | 0.41              |
| 1:E:18:LYS:HD3   | 1:E:18:LYS:N     | 2.35                     | 0.41              |
| 1:E:287:ILE:HG21 | 1:G:65:LEU:HG    | 1.99                     | 0.41              |
| 1:E:290:ARG:CD   | 1:G:64:ILE:HD13  | 2.38                     | 0.41              |
| 1:G:188:TYR:CE1  | 1:G:266:PHE:HB3  | 2.55                     | 0.41              |
| 1:H:111:ASN:HB3  | 1:H:116:ARG:HH21 | 1.85                     | 0.41              |
| 1:I:188:TYR:CE1  | 1:I:266:PHE:HB3  | 2.55                     | 0.41              |
| 1:J:296:ASN:HA   | 1:J:330:ILE:HD13 | 2.02                     | 0.41              |
| 1:K:111:ASN:HB3  | 1:K:116:ARG:HH21 | 1.85                     | 0.41              |
| 1:K:185:LEU:HB3  | 1:K:257:CYS:SG   | 2.60                     | 0.41              |
| 1:K:188:TYR:CE1  | 1:K:266:PHE:HB3  | 2.55                     | 0.41              |
| 1:B:185:LEU:HB3  | 1:B:257:CYS:SG   | 2.61                     | 0.41              |
| 1:B:221:LEU:HD22 | 1:B:221:LEU:H    | 1.86                     | 0.41              |
| 1:D:166:TYR:CD1  | 1:D:289:ILE:HG21 | 2.56                     | 0.41              |
| 1:D:188:TYR:CE1  | 1:D:266:PHE:HB3  | 2.55                     | 0.41              |
| 1:H:74:GLY:H     | 1:H:108:ALA:HB2  | 1.85                     | 0.41              |
| 1:I:185:LEU:HB3  | 1:I:257:CYS:SG   | 2.60                     | 0.41              |
| 1:I:221:LEU:H    | 1:I:221:LEU:HD22 | 1.85                     | 0.41              |
| 1:J:140:LEU:HD22 | 1:J:343:GLY:HA2  | 2.02                     | 0.41              |
| 1:K:18:LYS:HD3   | 1:K:18:LYS:N     | 2.35                     | 0.41              |
| 1:K:140:LEU:HD22 | 1:K:343:GLY:HA2  | 2.02                     | 0.41              |
| 1:K:335:ARG:HA   | 1:K:338:SER:HG   | 1.85                     | 0.41              |
| 1:A:370:VAL:O    | 1:A:374:CYS:HB2  | 2.21                     | 0.41              |
| 1:B:140:LEU:HD22 | 1:B:343:GLY:HA2  | 2.03                     | 0.41              |
| 1:C:49:GLN:HG3   | 1:C:49:GLN:O     | 2.20                     | 0.41              |
| 1:C:185:LEU:HB3  | 1:C:257:CYS:SG   | 2.60                     | 0.41              |
| 1:D:49:GLN:HG3   | 1:D:49:GLN:O     | 2.20                     | 0.41              |
| 1:E:49:GLN:O     | 1:E:49:GLN:HG3   | 2.20                     | 0.41              |
| 1:E:74:GLY:H     | 1:E:108:ALA:HB2  | 1.85                     | 0.41              |
| 1:E:185:LEU:HB3  | 1:E:257:CYS:SG   | 2.61                     | 0.41              |
| 1:E:370:VAL:O    | 1:E:374:CYS:HB2  | 2.21                     | 0.41              |
| 1:F:185:LEU:HB3  | 1:F:257:CYS:SG   | 2.60                     | 0.41              |
| 1:G:74:GLY:H     | 1:G:108:ALA:HB2  | 1.85                     | 0.41              |
| 1:G:185:LEU:HB3  | 1:G:257:CYS:SG   | 2.60                     | 0.41              |
| 1:G:370:VAL:O    | 1:G:374:CYS:HB2  | 2.21                     | 0.41              |
| 1:H:18:LYS:HG3   | 1:H:30:VAL:HG22  | 2.02                     | 0.41              |
| 1:H:49:GLN:O     | 1:H:49:GLN:HG3   | 2.20                     | 0.41              |
| 1:H:140:LEU:HD22 | 1:H:343:GLY:HA2  | 2.02                     | 0.41              |
| 1:H:166:TYR:CD1  | 1:H:289:ILE:HG21 | 2.56                     | 0.41              |
| 1:J:18:LYS:HG3   | 1:J:30:VAL:HG22  | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:18:LYS:HG3   | 1:B:30:VAL:HG22  | 2.02                     | 0.41              |
| 1:B:166:TYR:CD1  | 1:B:289:ILE:HG21 | 2.56                     | 0.41              |
| 1:B:370:VAL:O    | 1:B:374:CYS:HB2  | 2.21                     | 0.41              |
| 1:D:370:VAL:O    | 1:D:374:CYS:HB2  | 2.21                     | 0.41              |
| 1:E:18:LYS:HG3   | 1:E:30:VAL:HG22  | 2.02                     | 0.41              |
| 1:F:117:GLU:HG2  | 1:F:367:PRO:HG2  | 2.03                     | 0.41              |
| 1:F:166:TYR:CD1  | 1:F:289:ILE:HG21 | 2.56                     | 0.41              |
| 1:F:353:GLN:HA   | 1:F:356:TRP:HD1  | 1.84                     | 0.41              |
| 1:J:166:TYR:CD1  | 1:J:289:ILE:HG21 | 2.56                     | 0.41              |
| 1:J:370:VAL:O    | 1:J:374:CYS:HB2  | 2.21                     | 0.41              |
| 1:C:18:LYS:N     | 1:C:18:LYS:HD3   | 2.35                     | 0.41              |
| 1:C:111:ASN:HB3  | 1:C:116:ARG:HH21 | 1.85                     | 0.41              |
| 1:C:173:HIS:CE1  | 1:E:45:VAL:CG1   | 2.85                     | 0.41              |
| 1:D:368:SER:C    | 1:D:370:VAL:N    | 2.79                     | 0.41              |
| 1:E:188:TYR:CE1  | 1:E:266:PHE:HB3  | 2.55                     | 0.41              |
| 1:F:296:ASN:HA   | 1:F:330:ILE:HD13 | 2.02                     | 0.41              |
| 1:K:18:LYS:HG3   | 1:K:30:VAL:HG22  | 2.02                     | 0.41              |
| 1:K:368:SER:C    | 1:K:370:VAL:N    | 2.79                     | 0.41              |
| 1:B:18:LYS:HD3   | 1:B:18:LYS:N     | 2.35                     | 0.41              |
| 1:D:221:LEU:H    | 1:D:221:LEU:HD22 | 1.86                     | 0.41              |
| 1:F:221:LEU:H    | 1:F:221:LEU:HD22 | 1.86                     | 0.41              |
| 1:I:287:ILE:CD1  | 1:K:61:LYS:O     | 2.69                     | 0.41              |
| 1:I:296:ASN:HA   | 1:I:330:ILE:HD13 | 2.02                     | 0.41              |
| 1:I:370:VAL:O    | 1:I:374:CYS:HB2  | 2.21                     | 0.41              |
| 1:J:18:LYS:N     | 1:J:18:LYS:HD3   | 2.35                     | 0.41              |
| 1:J:151:ILE:HD13 | 1:J:278:THR:HG23 | 2.02                     | 0.41              |
| 1:K:221:LEU:HD22 | 1:K:221:LEU:H    | 1.86                     | 0.41              |
| 1:A:188:TYR:CE1  | 1:A:266:PHE:HB3  | 2.55                     | 0.41              |
| 1:A:287:ILE:CD1  | 1:C:61:LYS:O     | 2.69                     | 0.41              |
| 1:C:370:VAL:O    | 1:C:374:CYS:HB2  | 2.21                     | 0.41              |
| 1:D:31:PHE:HZ    | 1:D:89:THR:HG1   | 1.67                     | 0.41              |
| 1:D:98:PRO:O     | 1:D:129:VAL:HG12 | 2.21                     | 0.41              |
| 1:D:117:GLU:HG2  | 1:D:367:PRO:HG2  | 2.03                     | 0.41              |
| 1:D:193:LEU:HD23 | 1:D:253:GLU:HG2  | 2.03                     | 0.41              |
| 1:D:296:ASN:HA   | 1:D:330:ILE:HD13 | 2.02                     | 0.41              |
| 1:F:193:LEU:HD23 | 1:F:253:GLU:HG2  | 2.03                     | 0.41              |
| 1:F:312:ARG:HG3  | 1:F:312:ARG:NH1  | 2.33                     | 0.41              |
| 1:F:370:VAL:O    | 1:F:374:CYS:HB2  | 2.21                     | 0.41              |
| 1:H:221:LEU:H    | 1:H:221:LEU:HD22 | 1.86                     | 0.41              |
| 1:I:74:GLY:H     | 1:I:108:ALA:HB2  | 1.85                     | 0.41              |
| 1:K:166:TYR:CD1  | 1:K:289:ILE:HG21 | 2.56                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:151:ILE:HD13 | 1:A:278:THR:HG23 | 2.02                     | 0.41              |
| 1:B:12:ASN:HB3   | 1:B:71:ILE:CD1   | 2.51                     | 0.41              |
| 1:B:188:TYR:CE1  | 1:B:266:PHE:HB3  | 2.55                     | 0.41              |
| 1:B:287:ILE:CD1  | 1:D:61:LYS:O     | 2.69                     | 0.41              |
| 1:B:312:ARG:HG3  | 1:B:312:ARG:NH1  | 2.33                     | 0.41              |
| 1:C:74:GLY:H     | 1:C:108:ALA:HB2  | 1.85                     | 0.41              |
| 1:C:287:ILE:CD1  | 1:E:61:LYS:O     | 2.69                     | 0.41              |
| 1:D:18:LYS:HG3   | 1:D:30:VAL:HG22  | 2.02                     | 0.41              |
| 1:D:18:LYS:HD3   | 1:D:18:LYS:N     | 2.36                     | 0.41              |
| 1:D:151:ILE:HD13 | 1:D:278:THR:HG23 | 2.02                     | 0.41              |
| 1:D:287:ILE:CD1  | 1:F:61:LYS:O     | 2.69                     | 0.41              |
| 1:D:305:MET:O    | 1:D:306:TYR:C    | 2.64                     | 0.41              |
| 1:E:140:LEU:HD22 | 1:E:343:GLY:HA2  | 2.02                     | 0.41              |
| 1:F:18:LYS:HG3   | 1:F:30:VAL:HG22  | 2.02                     | 0.41              |
| 1:F:31:PHE:HZ    | 1:F:89:THR:HG1   | 1.67                     | 0.41              |
| 1:G:140:LEU:HD22 | 1:G:343:GLY:HA2  | 2.02                     | 0.41              |
| 1:G:296:ASN:HA   | 1:G:330:ILE:HD13 | 2.02                     | 0.41              |
| 1:H:117:GLU:HG2  | 1:H:367:PRO:HG2  | 2.03                     | 0.41              |
| 1:H:151:ILE:HD13 | 1:H:278:THR:HG23 | 2.02                     | 0.41              |
| 1:H:296:ASN:HA   | 1:H:330:ILE:HD13 | 2.02                     | 0.41              |
| 1:H:305:MET:O    | 1:H:306:TYR:C    | 2.64                     | 0.41              |
| 1:I:140:LEU:HD22 | 1:I:343:GLY:HA2  | 2.02                     | 0.41              |
| 1:J:185:LEU:HB3  | 1:J:257:CYS:SG   | 2.60                     | 0.41              |
| 1:J:353:GLN:HA   | 1:J:356:TRP:HD1  | 1.84                     | 0.41              |
| 1:K:49:GLN:O     | 1:K:49:GLN:HG3   | 2.20                     | 0.41              |
| 1:K:117:GLU:HG2  | 1:K:367:PRO:HG2  | 2.03                     | 0.41              |
| 1:K:151:ILE:HD13 | 1:K:278:THR:HG23 | 2.02                     | 0.41              |
| 1:K:305:MET:O    | 1:K:306:TYR:C    | 2.64                     | 0.41              |
| 1:A:185:LEU:HB3  | 1:A:257:CYS:SG   | 2.60                     | 0.41              |
| 1:B:49:GLN:O     | 1:B:49:GLN:HG3   | 2.20                     | 0.41              |
| 1:C:74:GLY:H     | 1:C:108:ALA:HB1  | 1.86                     | 0.41              |
| 1:C:140:LEU:HD22 | 1:C:343:GLY:HA2  | 2.02                     | 0.41              |
| 1:C:305:MET:O    | 1:C:306:TYR:C    | 2.64                     | 0.41              |
| 1:E:69:TYR:HA    | 1:E:70:PRO:HD2   | 1.95                     | 0.41              |
| 1:F:111:ASN:HB3  | 1:F:116:ARG:HH21 | 1.85                     | 0.41              |
| 1:F:151:ILE:HD13 | 1:F:278:THR:HG23 | 2.02                     | 0.41              |
| 1:G:173:HIS:CE1  | 1:I:45:VAL:CG1   | 2.85                     | 0.41              |
| 1:G:221:LEU:HD22 | 1:G:221:LEU:H    | 1.86                     | 0.41              |
| 1:G:305:MET:O    | 1:G:306:TYR:C    | 2.64                     | 0.41              |
| 1:G:335:ARG:HA   | 1:G:338:SER:HG   | 1.85                     | 0.41              |
| 1:H:18:LYS:N     | 1:H:18:LYS:HD3   | 2.35                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:185:LEU:HB3  | 1:H:257:CYS:SG   | 2.60                     | 0.41              |
| 1:H:193:LEU:HD23 | 1:H:253:GLU:HG2  | 2.03                     | 0.41              |
| 1:I:18:LYS:HG3   | 1:I:30:VAL:HG22  | 2.02                     | 0.41              |
| 1:I:353:GLN:HA   | 1:I:356:TRP:HD1  | 1.84                     | 0.41              |
| 1:K:296:ASN:HA   | 1:K:330:ILE:HD13 | 2.02                     | 0.41              |
| 1:K:353:GLN:HA   | 1:K:356:TRP:HD1  | 1.84                     | 0.41              |
| 1:B:117:GLU:HG2  | 1:B:367:PRO:HG2  | 2.03                     | 0.40              |
| 1:B:305:MET:O    | 1:B:306:TYR:C    | 2.64                     | 0.40              |
| 1:C:188:TYR:CE1  | 1:C:266:PHE:HB3  | 2.55                     | 0.40              |
| 1:C:353:GLN:HA   | 1:C:356:TRP:HD1  | 1.84                     | 0.40              |
| 1:E:287:ILE:CD1  | 1:G:61:LYS:O     | 2.69                     | 0.40              |
| 1:I:140:LEU:HD22 | 1:I:343:GLY:CA   | 2.52                     | 0.40              |
| 1:J:117:GLU:HG2  | 1:J:367:PRO:HG2  | 2.03                     | 0.40              |
| 1:J:305:MET:O    | 1:J:306:TYR:C    | 2.64                     | 0.40              |
| 1:A:18:LYS:HD3   | 1:A:18:LYS:N     | 2.36                     | 0.40              |
| 1:A:140:LEU:HD22 | 1:A:343:GLY:HA2  | 2.03                     | 0.40              |
| 1:B:151:ILE:HD13 | 1:B:278:THR:HG23 | 2.02                     | 0.40              |
| 1:B:368:SER:C    | 1:B:370:VAL:N    | 2.79                     | 0.40              |
| 1:C:166:TYR:CD1  | 1:C:289:ILE:HG21 | 2.55                     | 0.40              |
| 1:C:296:ASN:HA   | 1:C:330:ILE:HD13 | 2.02                     | 0.40              |
| 1:D:11:ASP:OD2   | 1:D:339:VAL:HG12 | 2.22                     | 0.40              |
| 1:D:12:ASN:HB3   | 1:D:71:ILE:CD1   | 2.51                     | 0.40              |
| 1:E:286:ASP:HB2  | 1:G:46:GLY:CA    | 2.52                     | 0.40              |
| 1:E:296:ASN:HA   | 1:E:330:ILE:HD13 | 2.02                     | 0.40              |
| 1:F:49:GLN:HG3   | 1:F:49:GLN:O     | 2.20                     | 0.40              |
| 1:F:355:MET:HE1  | 1:F:375:PHE:CE1  | 2.57                     | 0.40              |
| 1:I:98:PRO:O     | 1:I:129:VAL:HG12 | 2.21                     | 0.40              |
| 1:I:151:ILE:HD13 | 1:I:278:THR:HG23 | 2.02                     | 0.40              |
| 1:I:355:MET:HE1  | 1:I:375:PHE:CE1  | 2.57                     | 0.40              |
| 1:J:11:ASP:OD2   | 1:J:339:VAL:HG12 | 2.22                     | 0.40              |
| 1:J:140:LEU:HD22 | 1:J:343:GLY:CA   | 2.52                     | 0.40              |
| 1:A:221:LEU:H    | 1:A:221:LEU:HD22 | 1.85                     | 0.40              |
| 1:C:355:MET:HE1  | 1:C:375:PHE:CE1  | 2.57                     | 0.40              |
| 1:F:18:LYS:N     | 1:F:18:LYS:HD3   | 2.36                     | 0.40              |
| 1:F:98:PRO:O     | 1:F:129:VAL:HG12 | 2.21                     | 0.40              |
| 1:F:286:ASP:CB   | 1:H:46:GLY:C     | 2.91                     | 0.40              |
| 1:F:305:MET:O    | 1:F:306:TYR:C    | 2.64                     | 0.40              |
| 1:G:140:LEU:HD22 | 1:G:343:GLY:CA   | 2.52                     | 0.40              |
| 1:G:286:ASP:HB2  | 1:I:46:GLY:CA    | 2.52                     | 0.40              |
| 1:J:221:LEU:H    | 1:J:221:LEU:HD22 | 1.86                     | 0.40              |
| 1:K:12:ASN:HB3   | 1:K:71:ILE:CD1   | 2.51                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:140:LEU:HD22 | 1:K:343:GLY:CA   | 2.52                     | 0.40              |
| 1:K:370:VAL:O    | 1:K:374:CYS:HB2  | 2.21                     | 0.40              |
| 1:A:166:TYR:CD1  | 1:A:289:ILE:HG21 | 2.56                     | 0.40              |
| 1:B:98:PRO:O     | 1:B:129:VAL:HG12 | 2.21                     | 0.40              |
| 1:C:287:ILE:HD11 | 1:E:64:ILE:H     | 1.63                     | 0.40              |
| 1:C:368:SER:C    | 1:C:370:VAL:N    | 2.79                     | 0.40              |
| 1:D:312:ARG:HG3  | 1:D:312:ARG:NH1  | 2.33                     | 0.40              |
| 1:E:166:TYR:CD1  | 1:E:289:ILE:HG21 | 2.56                     | 0.40              |
| 1:G:12:ASN:HB3   | 1:G:71:ILE:CD1   | 2.51                     | 0.40              |
| 1:G:117:GLU:HG2  | 1:G:367:PRO:CG   | 2.52                     | 0.40              |
| 1:G:287:ILE:HD12 | 1:I:64:ILE:HD12  | 1.42                     | 0.40              |
| 1:H:353:GLN:HA   | 1:H:356:TRP:HD1  | 1.84                     | 0.40              |
| 1:H:370:VAL:O    | 1:H:374:CYS:HB2  | 2.21                     | 0.40              |
| 1:I:368:SER:C    | 1:I:370:VAL:N    | 2.79                     | 0.40              |
| 1:J:368:SER:C    | 1:J:370:VAL:N    | 2.79                     | 0.40              |
| 1:A:11:ASP:OD2   | 1:A:339:VAL:HG12 | 2.22                     | 0.40              |
| 1:A:12:ASN:HB3   | 1:A:71:ILE:CD1   | 2.51                     | 0.40              |
| 1:C:151:ILE:HD13 | 1:C:278:THR:HG23 | 2.02                     | 0.40              |
| 1:C:221:LEU:H    | 1:C:221:LEU:HD22 | 1.86                     | 0.40              |
| 1:F:287:ILE:HB   | 1:H:64:ILE:HG21  | 2.03                     | 0.40              |
| 1:F:287:ILE:CD1  | 1:H:61:LYS:O     | 2.69                     | 0.40              |
| 1:G:353:GLN:HA   | 1:G:356:TRP:HD1  | 1.84                     | 0.40              |
| 1:H:287:ILE:CD1  | 1:J:61:LYS:O     | 2.69                     | 0.40              |
| 1:I:166:TYR:CD1  | 1:I:289:ILE:HG21 | 2.56                     | 0.40              |
| 1:J:12:ASN:HB3   | 1:J:71:ILE:CD1   | 2.51                     | 0.40              |
| 1:J:98:PRO:O     | 1:J:129:VAL:HG12 | 2.21                     | 0.40              |
| 1:J:113:LYS:HD3  | 1:J:113:LYS:H    | 1.87                     | 0.40              |
| 1:K:98:PRO:O     | 1:K:129:VAL:HG12 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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     | 313/320 (98%)   | 310 (99%)  | 3 (1%)   | 68          | 78 |
| 1   | B     | 313/320 (98%)   | 310 (99%)  | 3 (1%)   | 68          | 78 |
| 1   | C     | 313/320 (98%)   | 310 (99%)  | 3 (1%)   | 68          | 78 |
| 1   | D     | 313/320 (98%)   | 310 (99%)  | 3 (1%)   | 68          | 78 |
| 1   | E     | 313/320 (98%)   | 310 (99%)  | 3 (1%)   | 68          | 78 |
| 1   | F     | 313/320 (98%)   | 310 (99%)  | 3 (1%)   | 68          | 78 |
| 1   | G     | 313/320 (98%)   | 310 (99%)  | 3 (1%)   | 68          | 78 |
| 1   | H     | 313/320 (98%)   | 310 (99%)  | 3 (1%)   | 68          | 78 |
| 1   | I     | 313/320 (98%)   | 310 (99%)  | 3 (1%)   | 68          | 78 |
| 1   | J     | 313/320 (98%)   | 310 (99%)  | 3 (1%)   | 68          | 78 |
| 1   | K     | 313/320 (98%)   | 310 (99%)  | 3 (1%)   | 68          | 78 |
| All | All   | 3443/3520 (98%) | 3410 (99%) | 33 (1%)  | 65          | 78 |

All (33) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 248 | ILE  |
| 1   | A     | 351 | THR  |
| 1   | A     | 364 | GLU  |
| 1   | B     | 248 | ILE  |
| 1   | B     | 351 | THR  |
| 1   | B     | 364 | GLU  |
| 1   | C     | 248 | ILE  |
| 1   | C     | 351 | THR  |
| 1   | C     | 364 | GLU  |
| 1   | D     | 248 | ILE  |
| 1   | D     | 351 | THR  |
| 1   | D     | 364 | GLU  |
| 1   | E     | 248 | ILE  |
| 1   | E     | 351 | THR  |
| 1   | E     | 364 | GLU  |
| 1   | F     | 248 | ILE  |
| 1   | F     | 351 | THR  |
| 1   | F     | 364 | GLU  |
| 1   | G     | 248 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 351 | THR  |
| 1   | G     | 364 | GLU  |
| 1   | H     | 248 | ILE  |
| 1   | H     | 351 | THR  |
| 1   | H     | 364 | GLU  |
| 1   | I     | 248 | ILE  |
| 1   | I     | 351 | THR  |
| 1   | I     | 364 | GLU  |
| 1   | J     | 248 | ILE  |
| 1   | J     | 351 | THR  |
| 1   | J     | 364 | GLU  |
| 1   | K     | 248 | ILE  |
| 1   | K     | 351 | THR  |
| 1   | K     | 364 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ASN  |
| 1   | A     | 88  | HIS  |
| 1   | A     | 92  | ASN  |
| 1   | A     | 111 | ASN  |
| 1   | A     | 173 | HIS  |
| 1   | A     | 354 | GLN  |
| 1   | A     | 371 | HIS  |
| 1   | B     | 12  | ASN  |
| 1   | B     | 88  | HIS  |
| 1   | B     | 92  | ASN  |
| 1   | B     | 111 | ASN  |
| 1   | B     | 173 | HIS  |
| 1   | B     | 354 | GLN  |
| 1   | C     | 12  | ASN  |
| 1   | C     | 88  | HIS  |
| 1   | C     | 92  | ASN  |
| 1   | C     | 111 | ASN  |
| 1   | C     | 173 | HIS  |
| 1   | C     | 354 | GLN  |
| 1   | C     | 371 | HIS  |
| 1   | D     | 12  | ASN  |
| 1   | D     | 88  | HIS  |
| 1   | D     | 92  | ASN  |
| 1   | D     | 111 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 173 | HIS  |
| 1   | D     | 354 | GLN  |
| 1   | E     | 12  | ASN  |
| 1   | E     | 40  | HIS  |
| 1   | E     | 88  | HIS  |
| 1   | E     | 92  | ASN  |
| 1   | E     | 111 | ASN  |
| 1   | E     | 173 | HIS  |
| 1   | E     | 354 | GLN  |
| 1   | E     | 371 | HIS  |
| 1   | F     | 12  | ASN  |
| 1   | F     | 88  | HIS  |
| 1   | F     | 92  | ASN  |
| 1   | F     | 111 | ASN  |
| 1   | F     | 173 | HIS  |
| 1   | F     | 354 | GLN  |
| 1   | F     | 371 | HIS  |
| 1   | G     | 12  | ASN  |
| 1   | G     | 40  | HIS  |
| 1   | G     | 88  | HIS  |
| 1   | G     | 92  | ASN  |
| 1   | G     | 111 | ASN  |
| 1   | G     | 173 | HIS  |
| 1   | G     | 354 | GLN  |
| 1   | H     | 12  | ASN  |
| 1   | H     | 88  | HIS  |
| 1   | H     | 92  | ASN  |
| 1   | H     | 111 | ASN  |
| 1   | H     | 173 | HIS  |
| 1   | H     | 354 | GLN  |
| 1   | I     | 12  | ASN  |
| 1   | I     | 88  | HIS  |
| 1   | I     | 92  | ASN  |
| 1   | I     | 111 | ASN  |
| 1   | I     | 173 | HIS  |
| 1   | I     | 354 | GLN  |
| 1   | I     | 371 | HIS  |
| 1   | J     | 12  | ASN  |
| 1   | J     | 88  | HIS  |
| 1   | J     | 92  | ASN  |
| 1   | J     | 111 | ASN  |
| 1   | J     | 354 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 371 | HIS  |
| 1   | K     | 12  | ASN  |
| 1   | K     | 88  | HIS  |
| 1   | K     | 92  | ASN  |
| 1   | K     | 111 | ASN  |
| 1   | K     | 354 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

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.

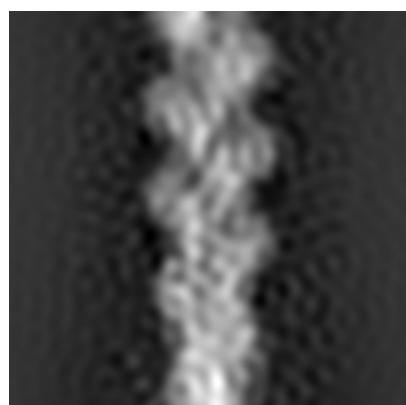
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6180. These allow visual inspection of the internal detail of the map and identification of artifacts.

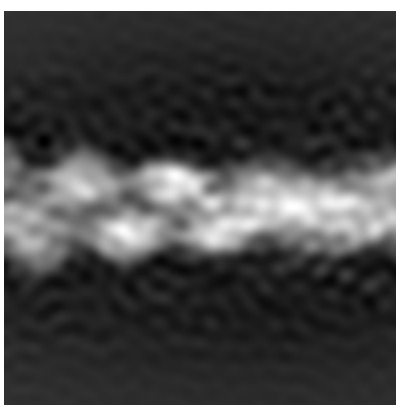
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

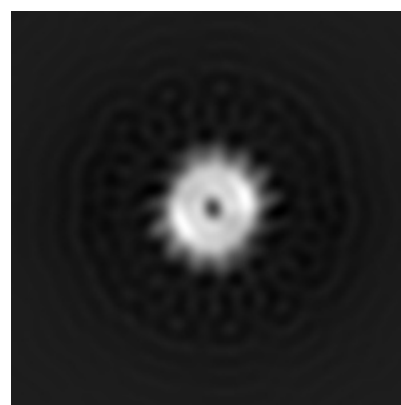
#### 6.1.1 Primary map



X



Y

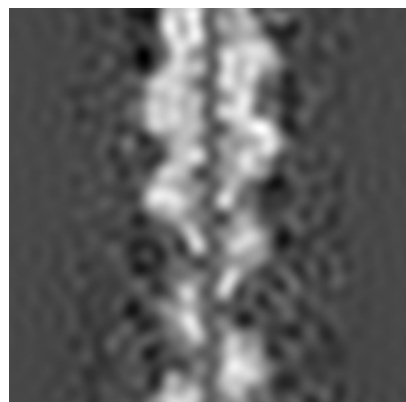


Z

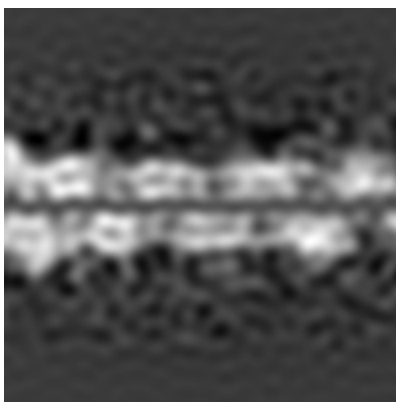
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

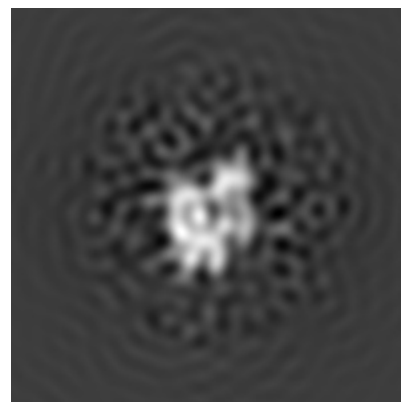
#### 6.2.1 Primary map



X Index: 50



Y Index: 50

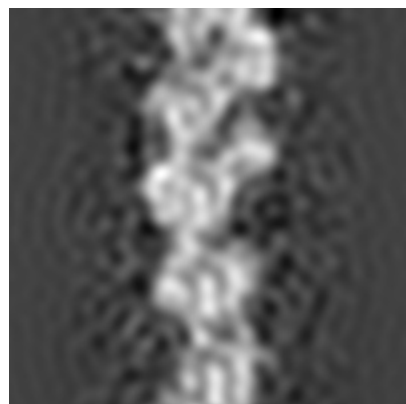


Z Index: 50

The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

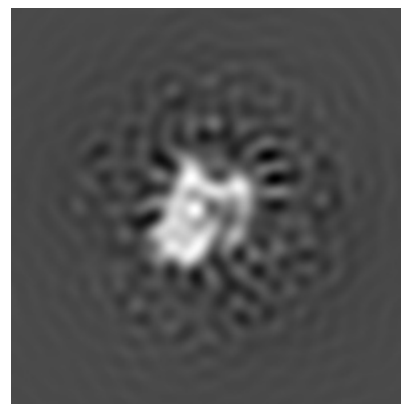
### 6.3.1 Primary map



X Index: 46



Y Index: 46

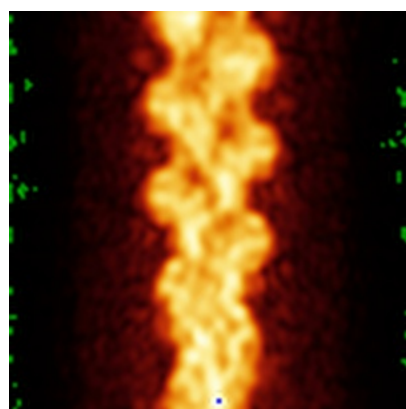


Z Index: 30

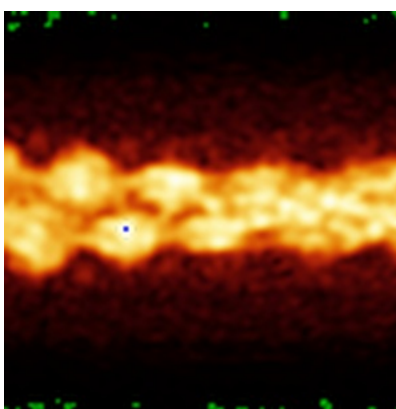
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

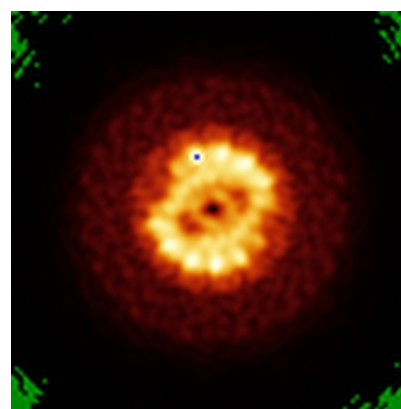
### 6.4.1 Primary map



X



Y

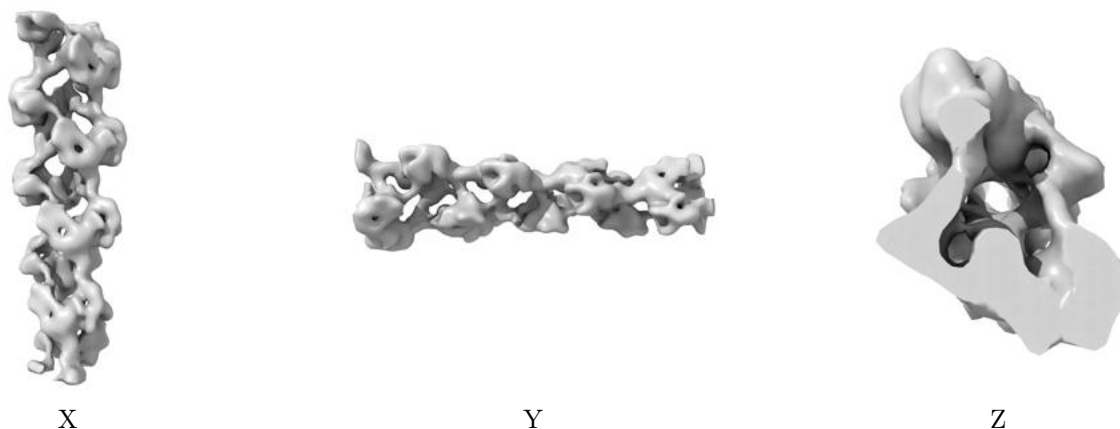


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

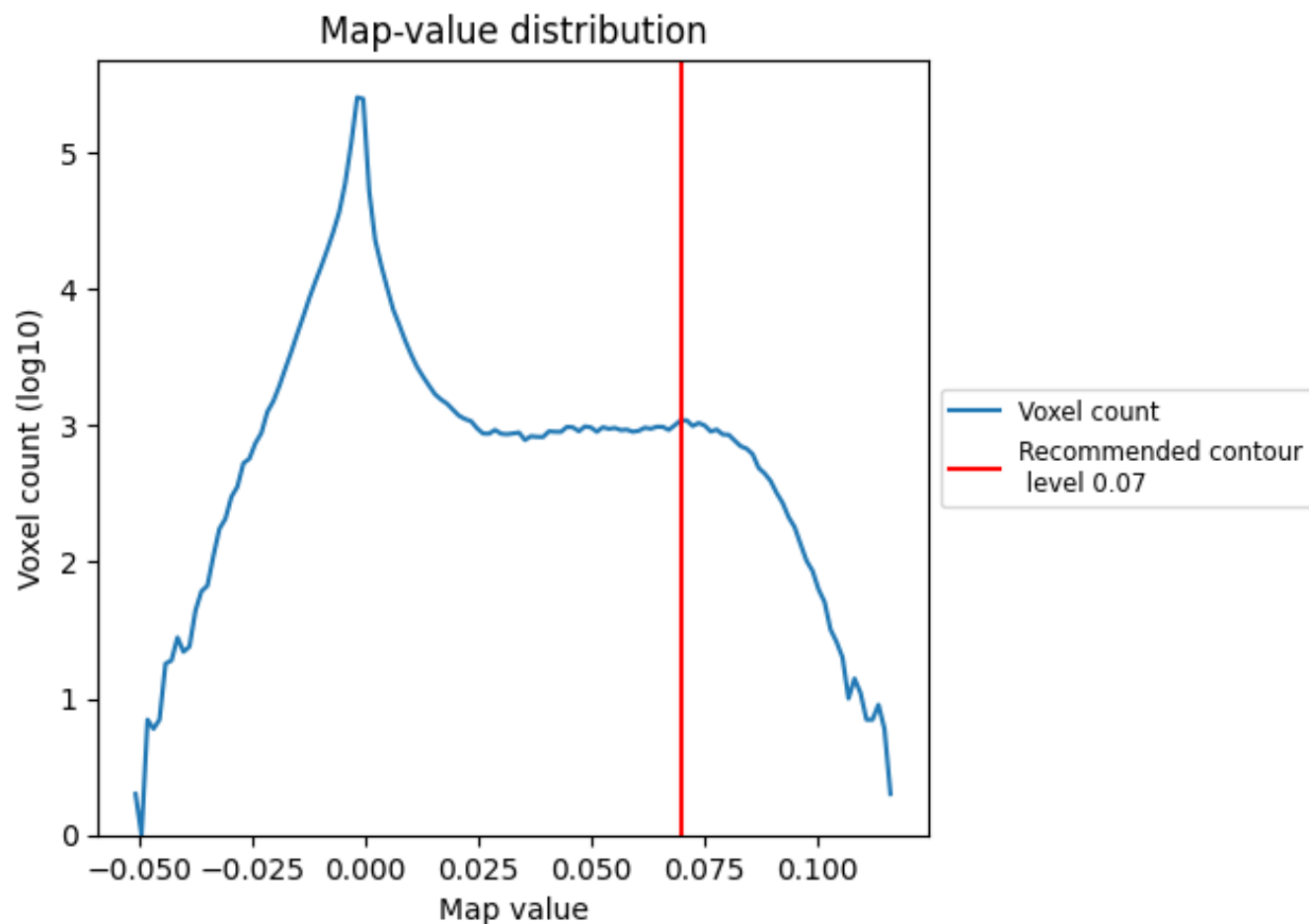
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

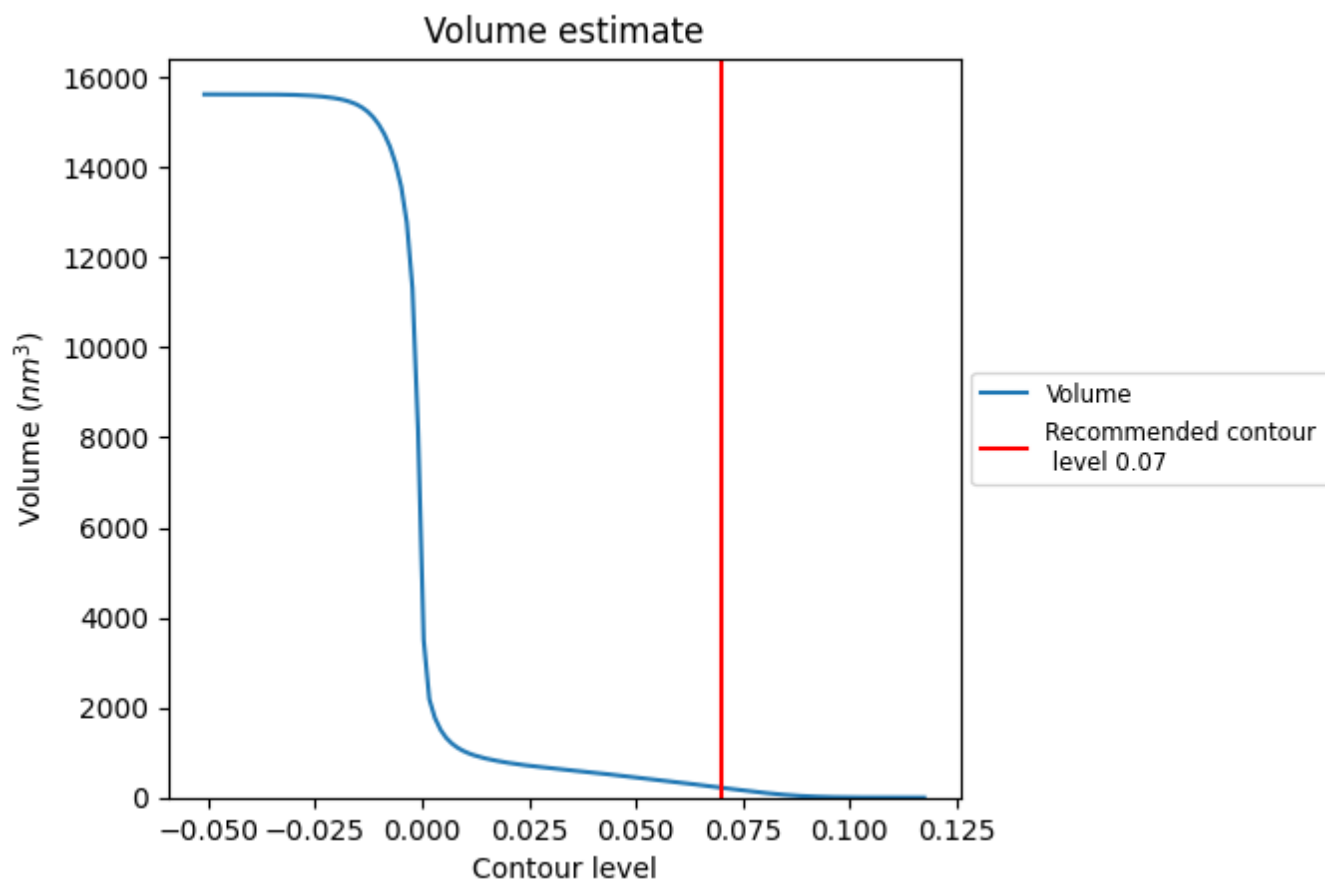
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

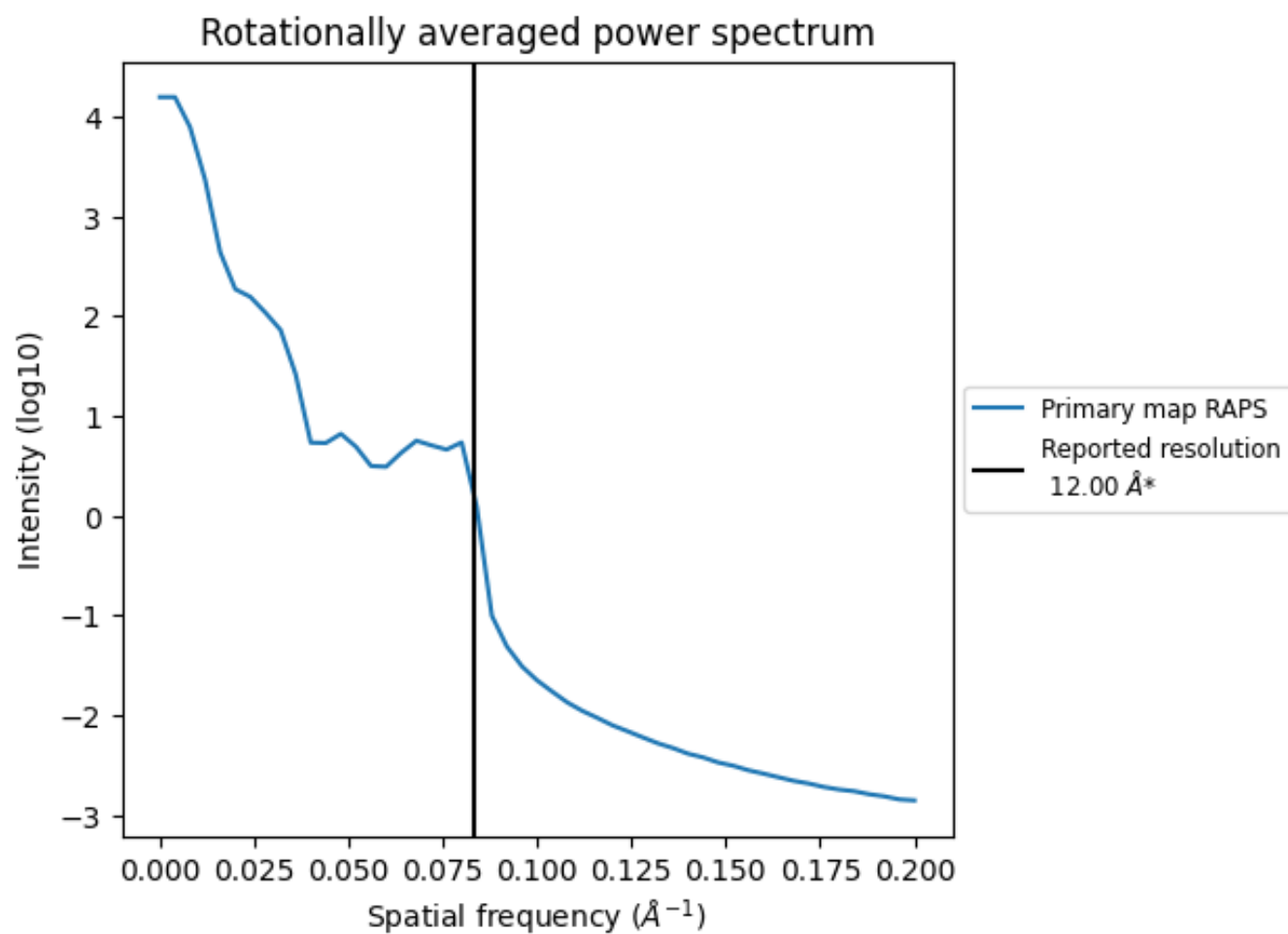
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 222 nm<sup>3</sup>; this corresponds to an approximate mass of 200 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.083 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

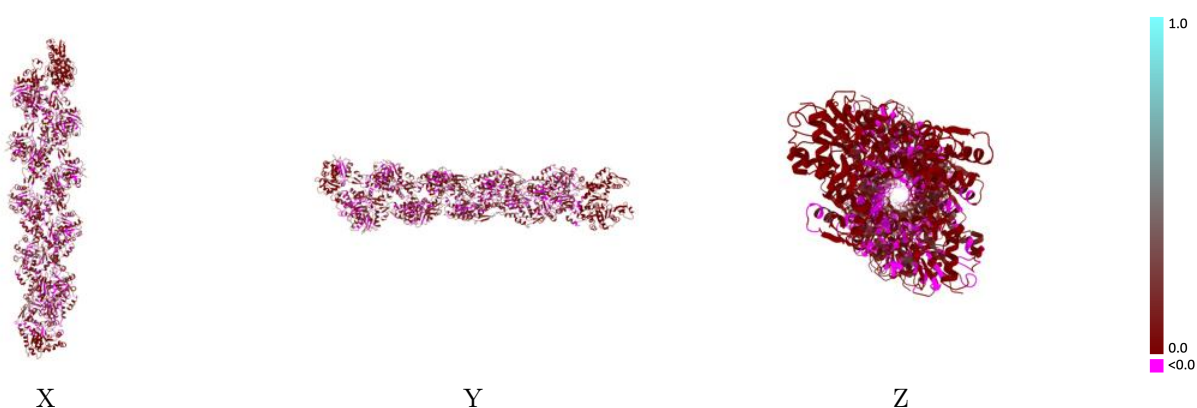
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6180 and PDB model 3J8J. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlay [i](#)

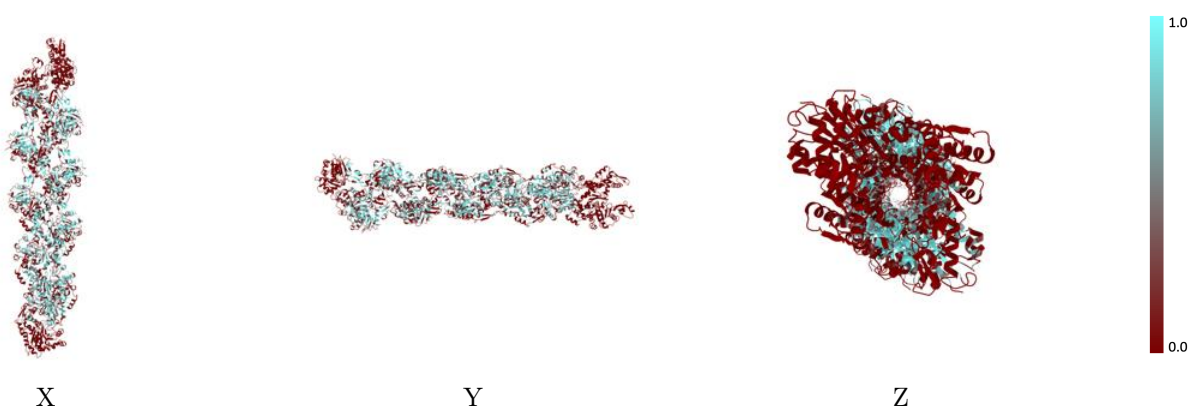
This section was not generated.

### 9.2 Q-score mapped to coordinate model [i](#)



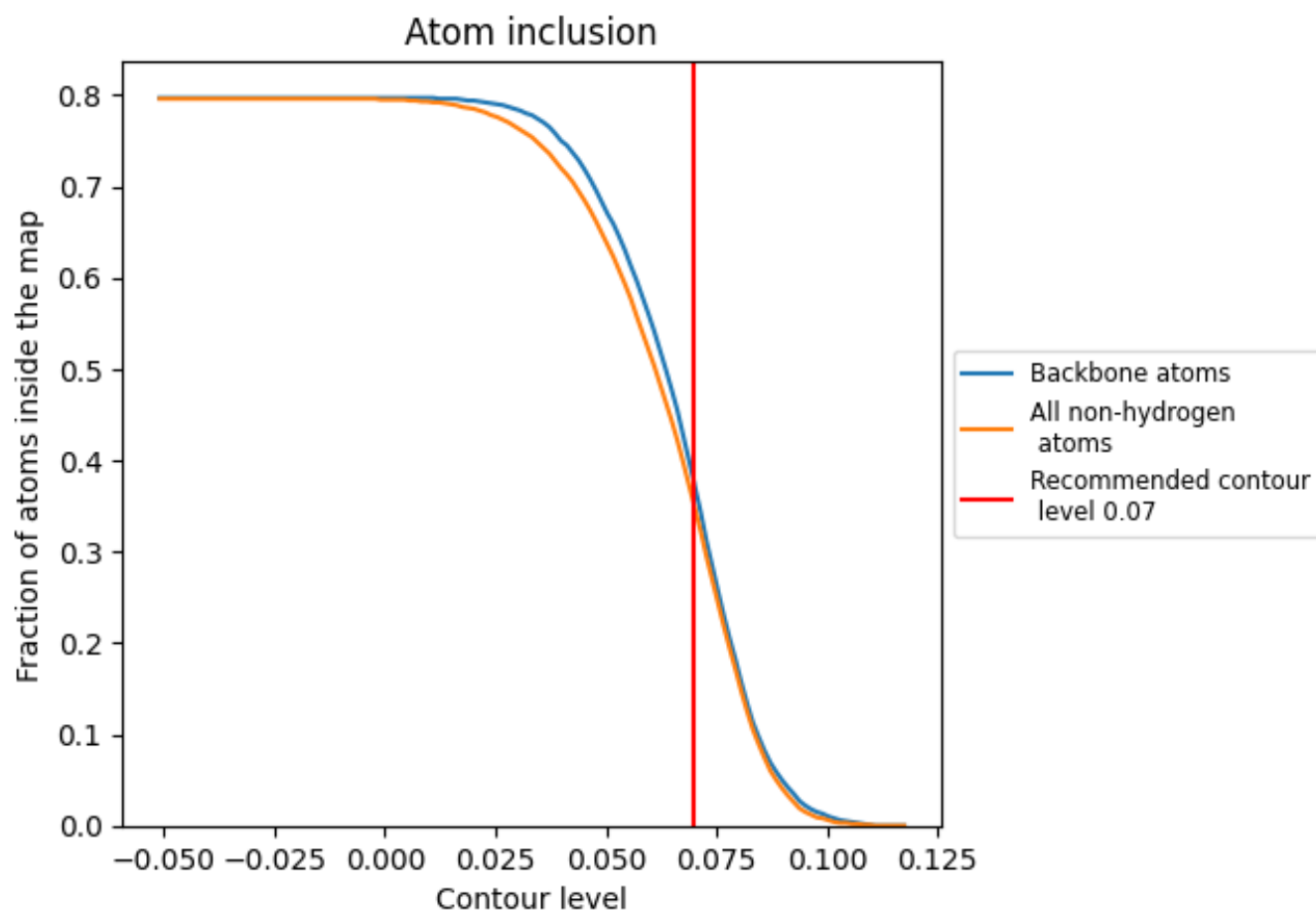
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 35% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                           | Q-score                                                                                   |
|-------|------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|
| All   |  0.3500 |  0.0610  |
| A     |  0.0050 |  -0.0010 |
| B     |  0.2470 |  0.0300  |
| C     |  0.4500 |  0.0750  |
| D     |  0.4170 |  0.0790  |
| E     |  0.4510 |  0.0770  |
| F     |  0.4240 |  0.0780  |
| G     |  0.4520 |  0.0810  |
| H     |  0.4170 |  0.0760  |
| I     |  0.4600 |  0.0820  |
| J     |  0.4150 |  0.0690  |
| K     |  0.1140 |  0.0220  |

