



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:27 am BST

PDB ID : 3DXJ  
Title : Crystal structure of thermus thermophilus rna polymerase holoenzyme in complex with the antibiotic myxopyronin  
Authors : Das, K.; Arnold, E.  
Deposited on : 2008-07-24  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | 1.8.5 (274361), CSD as541be (2020)                                 |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| buster-report                  | : | 1.1.7 (2018)   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

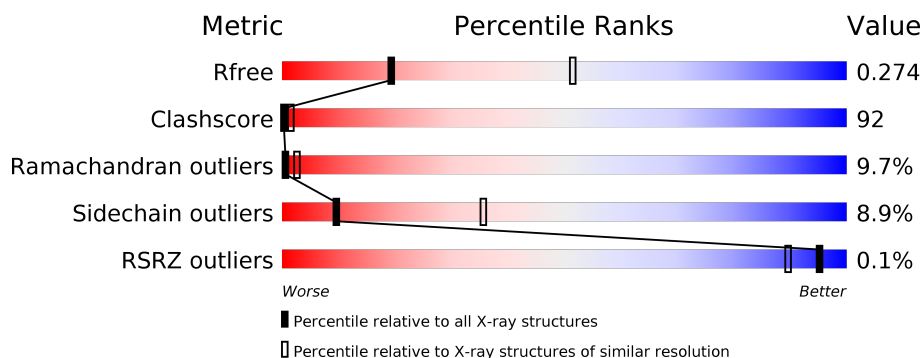
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 2092 (3.00-3.00)                                      |
| Clashscore            | 141614                      | 2416 (3.00-3.00)                                      |
| Ramachandran outliers | 138981                      | 2333 (3.00-3.00)                                      |
| Sidechain outliers    | 138945                      | 2336 (3.00-3.00)                                      |
| RSRZ outliers         | 127900                      | 1990 (3.00-3.00)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 315    |                  |
| 1   | B     | 315    |                  |
| 1   | K     | 315    |                  |
| 1   | L     | 315    |                  |
| 2   | C     | 1119   |                  |
| 2   | M     | 1119   |                  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | D     | 1524   |                  |
| 3   | N     | 1524   |                  |
| 4   | E     | 99     |                  |
| 4   | O     | 99     |                  |
| 5   | F     | 423    |                  |
| 5   | P     | 423    |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 10  | NE6  | D     | 1529 | X         | -        | -       | -                |
| 10  | NE6  | N     | 1528 | X         | -        | -       | -                |

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 56149 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1816  | 1159 | 315 | 339 | 3 |         |         |       |
| 1   | B     | 243      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1902  | 1212 | 328 | 359 | 3 |         |         |       |
| 1   | K     | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1816  | 1159 | 315 | 339 | 3 |         |         |       |
| 1   | L     | 243      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1902  | 1212 | 328 | 359 | 3 |         |         |       |

- Molecule 2 is a protein called BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | C     | 1119     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8829  | 5581 | 1577 | 1647 | 24 |         |         |       |
| 2   | M     | 1119     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8829  | 5581 | 1577 | 1647 | 24 |         |         |       |

- Molecule 3 is a protein called BACTERIAL RNA POLYMERASE BETA-PRIME SUBUNIT; CHAIN D, N.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | D     | 1504     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11864 | 7518 | 2091 | 2219 | 36 |         |         |       |
| 3   | N     | 1504     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11864 | 7518 | 2091 | 2219 | 36 |         |         |       |

- Molecule 4 is a protein called BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 488 | 133 | 144 | 4 |         |         |       |
| 4   | O     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 488 | 133 | 144 | 4 |         |         |       |

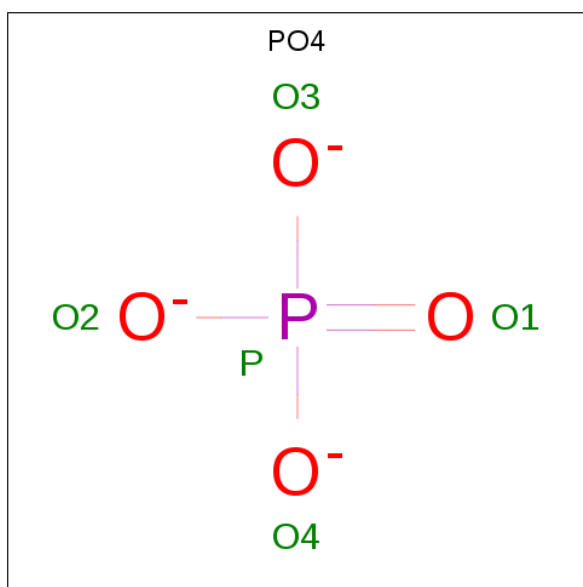
There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| E     | 61      | GLU      | VAL    | VARIANT | UNP Q8RQE7 |
| E     | 92      | ILE      | LEU    | VARIANT | UNP Q8RQE7 |
| E     | 95      | GLY      | VAL    | VARIANT | UNP Q8RQE7 |
| O     | 61      | GLU      | VAL    | VARIANT | UNP Q8RQE7 |
| O     | 92      | ILE      | LEU    | VARIANT | UNP Q8RQE7 |
| O     | 95      | GLY      | VAL    | VARIANT | UNP Q8RQE7 |

- Molecule 5 is a protein called RNA polymerase principal sigma factor (RpoD); CHAIN F, P.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | F     | 349      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2829  | 1785 | 513 | 527 | 4 |         |         |       |
| 5   | P     | 349      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2829  | 1785 | 513 | 527 | 4 |         |         |       |

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

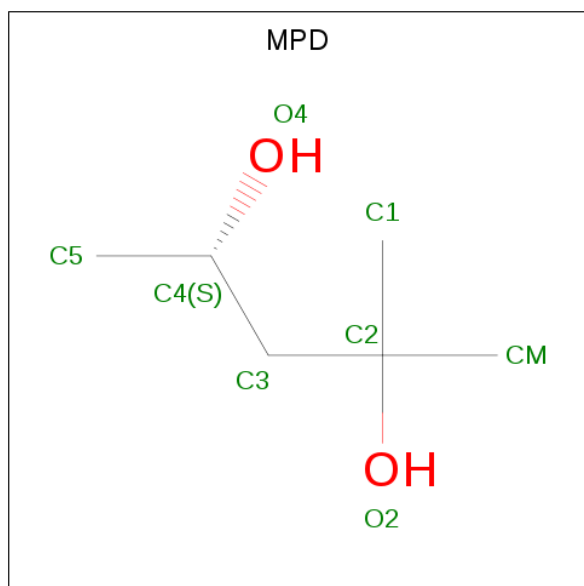


| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 6   | A     | 1        | Total O P<br>5 4 1 | 0       | 0       |
| 6   | D     | 1        | Total O P<br>5 4 1 | 0       | 0       |

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 7   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 7   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 7   | N     | 1        | Total Mg<br>1 1 | 0       | 0       |

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).

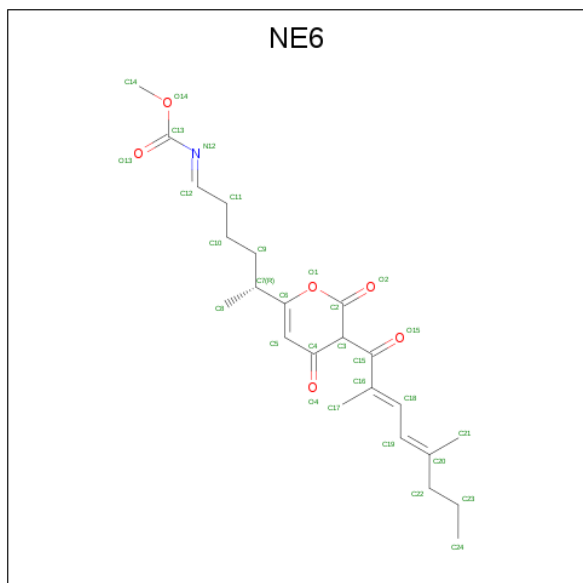


| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 8   | C     | 1        | Total C O<br>8 6 2 | 0       | 0       |
| 8   | C     | 1        | Total C O<br>8 6 2 | 0       | 0       |
| 8   | M     | 1        | Total C O<br>8 6 2 | 0       | 0       |

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | D     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 9   | N     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 10 is methyl [(1E,5R)-5-{(3S)-3-[(2E,4E)-2,5-dimethylocta-2,4-dienoyl]-2,4-dihydro-3,4-dihydro-2H-pyran-6-yl}hexylidene]carbamate (three-letter code: NE6) (formula: C<sub>23</sub>H<sub>31</sub>NO<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 10  | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 30    | 23 | 1 | 6 |         |         |
| 10  | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 30    | 23 | 1 | 6 |         |         |

- Molecule 11 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 11  | A     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 11  | B     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 11  | C     | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 11  | D     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 11  | F     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

*Continued on next page...*

*Continued from previous page...*

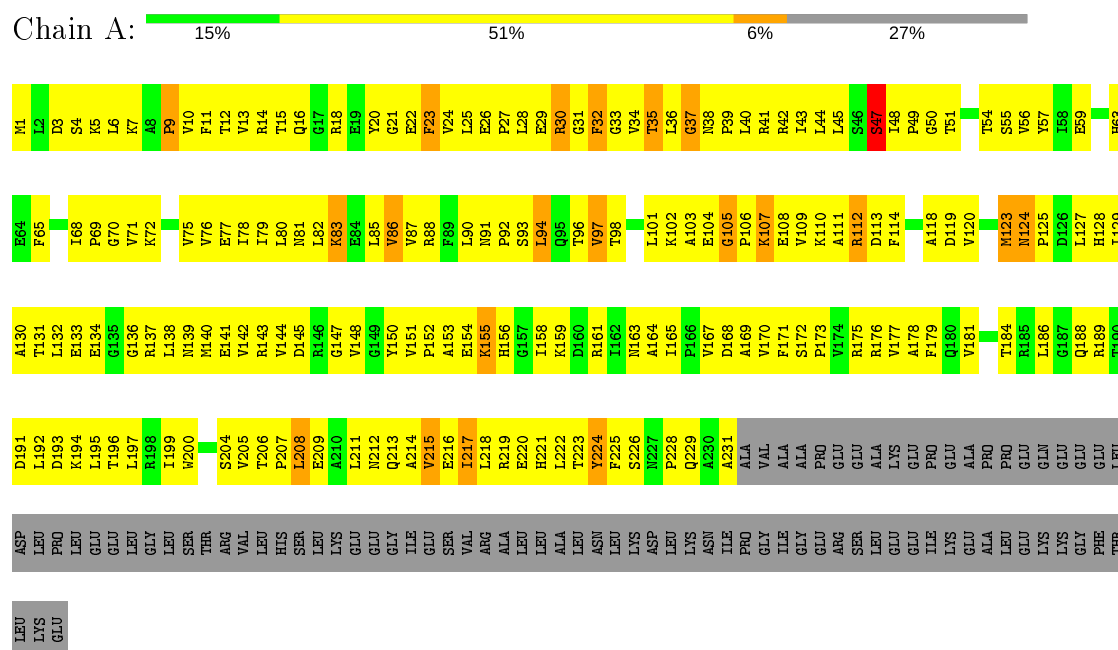
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 11  | M     | 5        | Total<br>5 | O<br>5 | 0       | 0       |
| 11  | N     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 11  | O     | 1        | Total<br>1 | O<br>1 | 0       | 0       |



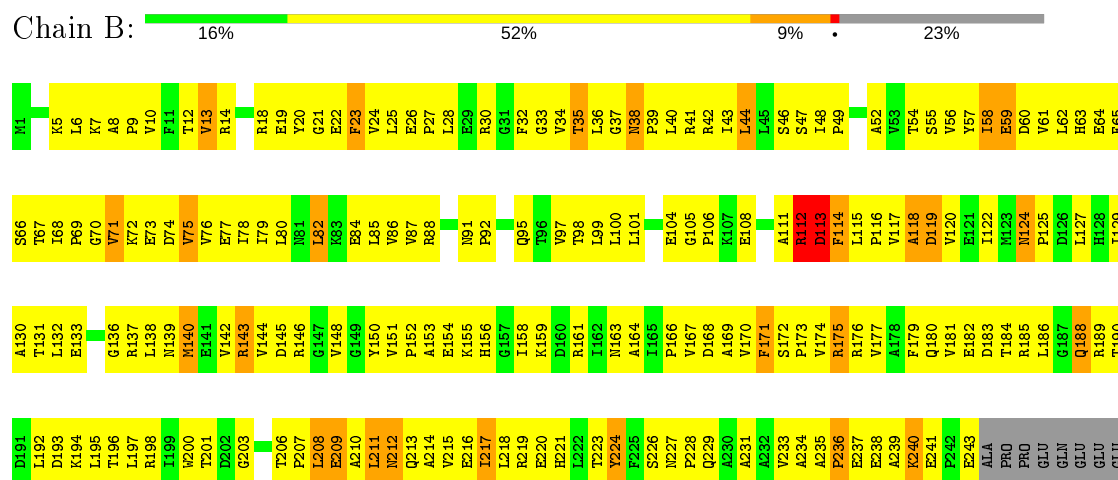
### 3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L

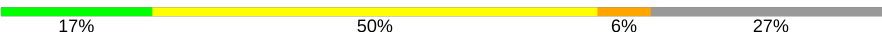


- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L



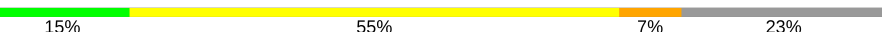
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| LEU | ASP | LEU | PRO | LEU | GLU | GLU | GLY | SER | THR | ARG | VAL | LEU | HIS | SER | LEU | LYS | GLU | GLY | ILE | GLU | SER | VAL | ARG | ALA | LEU | LEU | ALA | LEU | ASN | LEU | LYS | ASP | LEU | LYS | LYS | ASN | ILE | PRO | GLY | ILE | GLY | GLU | ARG | SER | LEU | GLU | ILE | LYS | ALA | LEU | GLU | LYS | LYS | PHE |
| THR | LEU | LYS | GLU |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |

- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L

Chain K: 

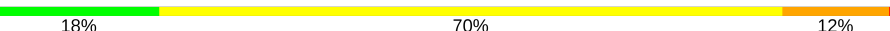
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|
| M1   | M2   | D3   | S4   | K5   | K7   | P9   | F10  | F11  | T12  | V13  | R14  | R18  | E19  | V20  | G21  | E22  | F23  | V24  | L25  | E26  | P27  | L28  | E29  | R30  | G31  | F32  | G33  | V34  | T35  | L36  | G37  | N38  | P39  | L40  | R41  | R42  | L43  | L44  | L45  | S46  | S47  | L48  | P49  | V53  | T54  | S55  | V56  | Y57  | I58  | E59  | H63  | E64 | F65 | L66 |     |     |
| T67  | L68  | P69  | G70  | V71  | K72  | E73  | D74  | V75  | V76  | E77  | V78  | I79  | L80  | N81  | L82  | V86  | R87  | R88  | F89  | L90  | L94  | V97  | T98  | L99  | L100 | L101 | K102 | A103 | A104 | G105 | P106 | K107 | E108 | V109 | K110 | A111 | R112 | D113 | F114 | L115 | A118 | D119 | V120 | E121 | I122 | M123 | V124 | S55  | V56  | Y57  | I58  | E59 | H63 | E64 | F65 | L66 |
| E133 | E134 | L138 | M139 | M140 | E141 | V142 | R143 | R146 | G147 | V148 | V151 | P152 | A153 | E154 | K155 | H156 | G157 | I158 | I162 | M163 | A164 | P166 | V167 | D168 | A169 | V170 | P173 | V174 | R175 | R176 | V177 | A178 | F179 | V181 | Q180 | D182 | T184 | R185 | L186 | G187 | R188 | T189 | D191 | L192 | D193 | L194 | T195 | T196 | L197 | R198 | I199 |     |     |     |     |     |
| T200 | T201 | D202 | G203 | S204 | V205 | T206 | P207 | L208 | E209 | L210 | L211 | Q212 | Q213 | V215 | E216 | L217 | L218 | R219 | E220 | E221 | L222 | T223 | V224 | F225 | S226 | N227 | P228 | Q229 | A230 | A231 | ALA  | VAL  | ALA  | ALA  | PRO  | GLU  | GLU  | GLU  | GLU  | ALA  | PRO  | PRO  | GLU  | GLN  | GLU  | GLU  | GLU  | GLU  | THR  | ASP  | LEU  | LEU | PRO | LEU | GLU | LEU |
| GLY  | LEU  | SER  | THR  | ARG  | VAL  | LEU  | HIS  | SER  | LEU  | LYS  | GLU  | GLY  | ILE  | GLU  | SER  | VAL  | ALA  | ALA  | LEU  | LEU  | ASN  | LEU  | LEU  | LYS  | ASP  | LEU  | LYS  | ASN  | ILE  | PRO  | GLY  | ILE  | GLU  | GLU  | ARG  | SER  | LEU  | GLU  | GLU  | ILE  | LYS  | GLU  | ALA  | ALA  | LEU  | GLU  | LYS  | PHE  | THR  | LEU  | LYS  | GLU | LEU | GLU | LEU |     |

- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L

Chain L: 

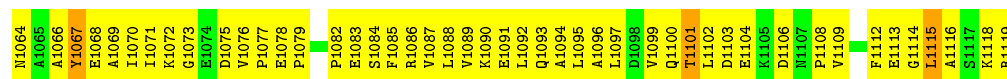
|     |     |      |      |      |     |
|-----|-----|------|------|------|-----|
| GLU | PRO | R189 | I129 | P69  | M1  |
|     | LEU | T190 | A130 | G70  | K5  |
|     | GLU | D193 | T131 | V71  | L6  |
|     | LEU | K194 | L132 | K72  | K7  |
|     | GLY | L195 | E133 | E73  | L8  |
|     | LEU | T196 | G135 | D74  | P9  |
|     | SER | L197 | G136 | V75  | V10 |
|     | THR | R198 | R137 | V76  | F11 |
|     | ARG | I199 | L138 | I78  | T12 |
|     | VAL | W200 | M139 | I79  | V13 |
|     | LEU | T201 | M140 | L80  | R14 |
|     | HIS | D202 | E141 | R81  |     |
|     | SER | G203 | V142 | L82  | R18 |
|     | LEU | S204 | R143 | K83  | E19 |
|     | LYS | V205 | V144 | E84  | Y20 |
|     | GLU | T206 | D145 | L85  | G21 |
|     | GLY | P207 | R146 | V86  | E22 |
|     | ILE | E209 | G147 | V87  | F23 |
|     | GLU | A210 | V148 | R88  | V24 |
|     | SER | L211 | G149 | F89  | L25 |
|     | VAL | N212 | V150 | L90  | E26 |
|     | ARG | Q213 | V151 | N91  | P27 |
|     | ALA | A214 | P152 | P92  | L28 |
|     | LEU | V215 | A153 | S93  | E29 |
|     | LEU | E216 | E154 | L94  | R30 |
|     | ALA | I217 | K155 | Q95  | G31 |
|     | LEU | L218 | H156 | T96  | F32 |
|     | ASN | R219 | V157 | V97  | G33 |
|     | LEU | E220 | I158 | T98  | V34 |
|     | ASP | H221 | K159 | L99  | T35 |
|     | LEU | Y224 | D160 | L100 | L36 |
|     | LYS | F225 | R161 | L101 | G37 |
|     | LEU | S226 | I162 | K102 | N38 |
|     | ASN | N227 | M163 | A103 | P39 |
|     | ILE | P228 | A164 | E104 | L40 |
|     | GLY | Q229 | I165 | G105 | R41 |
|     | ILE | V233 | P166 | P106 | R42 |
|     | GLY | A234 | V167 | K107 | L43 |
|     | GLY | E241 | D168 | E108 | L44 |
|     | GLU | P242 | A169 | V109 |     |
|     | GLU | ALA  | V170 | K110 | S47 |
|     | ARG | A235 | F171 | A111 | L48 |
|     | SER | P236 | S172 | R112 |     |
|     | LEU | K240 | P173 | D113 | A52 |
|     | GLU | E241 | V174 | F114 | V53 |
|     | ILE | P242 | R175 | L115 | T54 |
|     | LYS | E243 | R176 | P116 | S55 |
|     | GLU | ALA  | V177 | V117 | V56 |
|     | ALA | PRO  | A178 | D118 | Y57 |
|     | LEU | PRO  | F179 | A119 | I58 |
|     | LEU | GLU  | Q180 | V120 | E59 |
|     | LYS | GLU  | V181 | E121 | D60 |
|     | LYS | GLN  | E182 | I122 | V61 |
|     | LYS | GLU  | D183 | M123 |     |
|     | GLY | GLU  | T184 | N124 | E64 |
|     | PHE | GLU  | R185 | P125 | F65 |
|     | THR | LEU  | L186 | D126 | S66 |
|     | LEU | ASP  | G187 | L127 | T67 |
|     | LYS | LEU  | Q188 | H128 | L68 |

- Molecule 2: BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M

Chain C: 

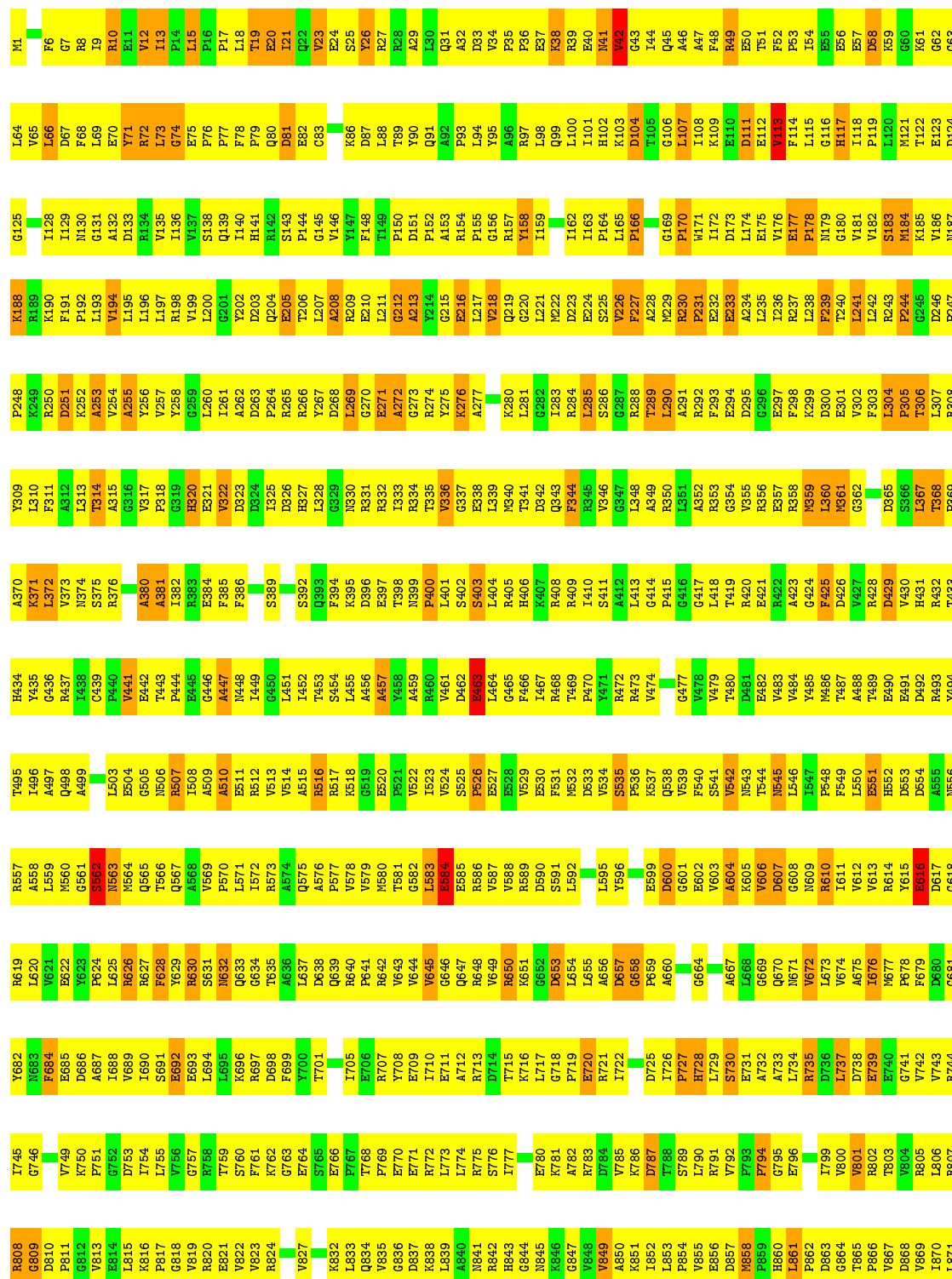
|    |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | E2 | I3 | K4 | R5 | F6 | G7 | R8 | I9 | E11 | L12 | V13 | I14 | F15 | P16 | P17 | L18 | T19 | E20 | Q22 | V23 | E24 | S25 | V26 | R27 | L30 | Q31 | A32 | D33 | V34 | P35 | P36 | E37 | K38 | R39 | E40 | N41 | V42 | G43 | I44 | Q45 | A46 | A47 | F48 | R49 | E50 | T51 | F52 | P53 | I54 | E55 | E56 | E57 | D58 | K59 | G60 | K61 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|





● Molecule 2: BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M

Chain M: 17% 69% 13%



|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G1062 | R1063 | N1064 | A1065 | A1066 | Y1067 | E1068 | A1069 | I1070 | K1071 | K1072 | G1073 | D1074 | D1075 | V1076 | P1077 | E1078 | P1079 | S1080 | V1081 | P1082 | E1083 | S1084 | F1085 | R1086 | V1087 | L1088 | V1089 | K1090 | E1091 | L1092 | Q1093 | A1094 | L1095 | A1096 | L1097 | D1098 | V1099 | Q1100 | T1101 | L1102 | D1103 | E1104 | K1105 | D1106 | M1107 | P1108 | V1109 | D1110 | F1111 | F1112 | E1113 | G1114 | L1115 | A1116 | S1117 | K1118 | R1119 |       |
| M1000 | V1001 | E1002 | D1003 | K1004 | M1005 | H1006 | A1007 | R1008 | S1009 | T1010 | G1011 | P1012 | S1013 | S1014 | L1015 | T1016 | Q1017 | Q1018 | Q1019 | P1020 | L1021 | G1022 | G1023 | Q1026 | F1027 | G1028 | G1029 | Q1030 | L1031 | F1032 | G1033 | A1034 | M1035 | L1036 | V1037 | H1038 | A1039 | L1040 | E1041 | A1042 | A1044 | A1045 | A1046 | H1047 | T1048 | L1049 | Q1050 | E1051 | M1052 | L1053 | L1054 | L1055 | K1056 | S1057 | D1058 | I1059 | I1060 | E1061 |
| G933  | F934  | D937  | K938  | R939  | E940  | V941  | E942  | V943  | L944  | R945  | R946  | A947  | E948  | K949  | V953  | K957  | T958  | P959  | G960  | E961  | Q962  | L963  | Q969  | G970  | K971  | L974  | Y975  | D976  | G977  | R978  | T979  | G980  | I981  | P982  | E983  | L984  | E985  | P986  | I987  | V988  | G989  | G990  | Y991  | F992  | F993  | K996  | L997  | Y998  | H999  |       |       |       |       |       |       |       |       |       |
| L872  | P873  | L874  | G875  | V876  | P877  | S878  | R879  | R880  | R881  | Q884  | L885  | L886  | E887  | T888  | H889  | L890  | G891  | L892  | A893  | G894  | Y895  | F896  | L897  | G898  | Q899  | R900  | Y901  | I902  | S903  | P904  | I905  | F906  | D907  | G908  | A909  | K910  | E911  | P912  | E913  | I914  | K915  | E916  | L917  | L918  | A919  | P986  | A921  | P922  | E923  | V924  | Y925  | F926  | Y927  | K928  | R929  | R930  | G931  | E932  |

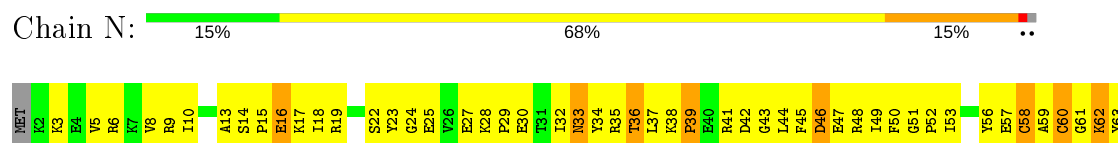
• Molecule 3: BACTERIAL RNA POLYMERASE BETA-PRIME SUBUNIT; CHAIN D, N

Chain D:  15% 69% 14%

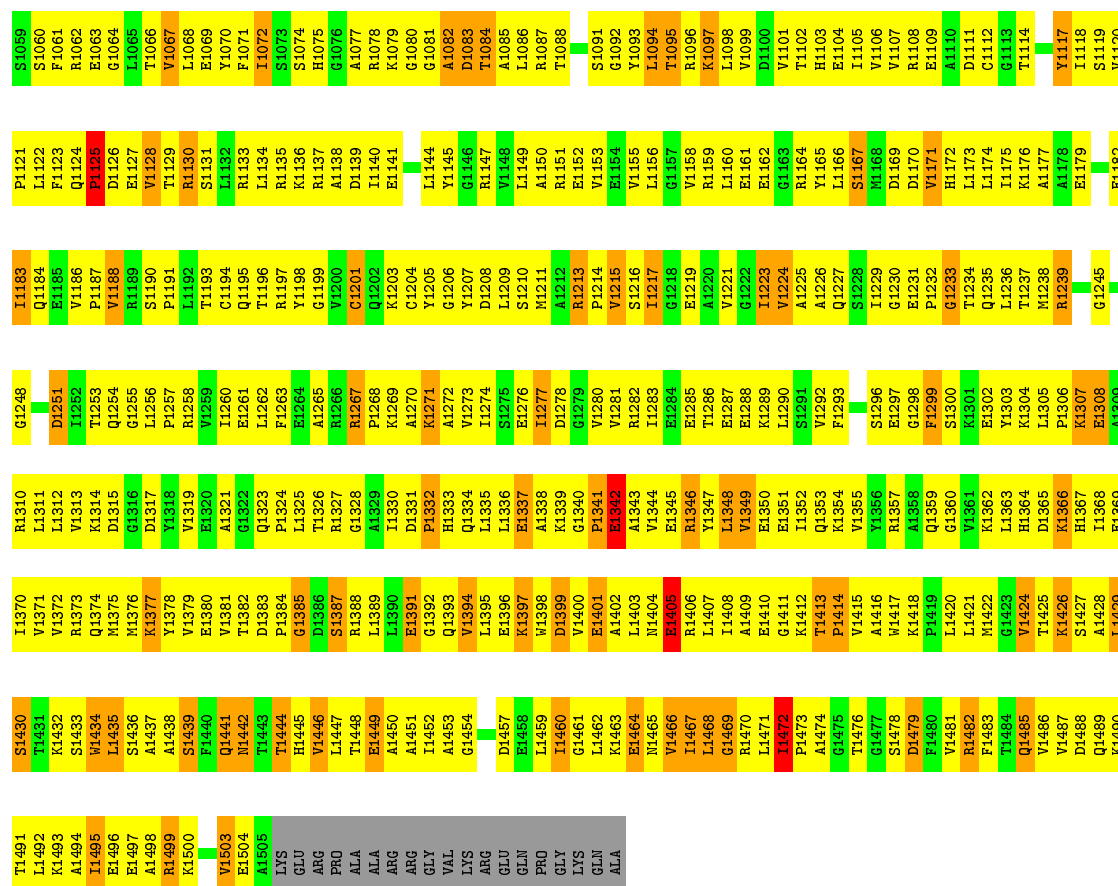
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| R615 | K616 | M617 | L618 | L619 | G620 | Q621 | R622 | G623 | P624 | P625 | S626 | G627 | R628 | S629 | V630 | L631 | P632 | G633 | M634 | L635 | Q636 | L637 | L638 | L639 | H640 | Q641 | L642 | L643 | L644 | P645 | L646 | R647 | L648 | L649 | L650 | E651 | T652 | P653 | K654 | P655 | G656 | L657 | L658 | K659 | L660 | L661 | G662 | L663 | L664 | L665 | L666 | L667 | L668 | L669 | V670 | K671 | G672 | A673 | R674 |
| K494 | R434 | I371 | K308 | E247 | E183 | T121 | K61  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| K495 | V435 | P372 | G309 | P248 | E184 | E122 | K62  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| K496 | E436 | P373 | L310 | Y249 | V185 | L123 | V63  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| E497 | V437 | E374 | L311 | L250 | V186 | E124 | K64  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| V498 | D438 | E375 | R312 | F251 | K187 | Q125 | R65  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| V499 | L439 | E376 | K313 | R252 | G188 | V126 | R66  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| R500 | V440 | P377 | P314 | A253 | Q189 | L127 | F67  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| A501 | R441 | I378 | R315 | E254 | E190 | K128 | R78  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| F502 | M442 | A379 | Q316 | E255 | L191 | F129 | R69  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| L503 | K443 | E380 | V317 | E256 | A192 | S130 | I10  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| D504 | R444 |      | R318 | G257 | P193 | K131 | A11  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| S505 | V445 | V384 | A319 | V258 | G194 | V132 | L12  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| G506 | V446 | V385 |      | V259 | V195 | I133 | A13  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| N507 | V447 | H386 | V322 | E260 | R198 | V134 | S14  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| R508 | E448 | L387 | E323 | L261 | K198 | L135 | R75  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| P509 | S449 | H388 | A324 | K262 | L199 | D136 | P15  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| E510 | Y450 | E389 | E325 | E263 | D200 | P137 | K17  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| M511 | D451 | P390 | E326 | L264 |      | K138 | I18  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| P512 | L452 | A391 | E327 | E265 | A203 | G139 | R19  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| K573 | D453 | S392 | G328 | E266 | L204 | A140 | S20  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| L514 | R454 | I393 | E329 | G267 | Y205 | E141 | W21  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| E515 | A455 | L394 | T330 | A268 | R206 | L142 | S22  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| A516 | M456 | V395 | V331 | F269 | F207 | N143 | Y23  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| V517 | G457 | V396 | V332 | L270 | F208 | G144 | G24  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| P518 | L458 | K397 | L333 | V271 | R209 | V145 | E25  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| V519 | E459 | A398 | T334 | L272 | R210 | P146 | V26  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| L520 | A460 | R399 | L335 | R273 | V211 | E147 | K28  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| P521 | I461 | V401 | F336 | R274 | R212 | K148 | P29  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| E522 | Q462 | Y401 | L337 |      | K149 | E150 | E30  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| D523 | Q463 | P402 | E338 | E277 | E214 | R150 | T31  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| L524 | L464 | F403 | V339 | P278 | Y215 | Q151 | G91  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| R525 | L465 | E404 | T340 | V279 | V216 | L152 | H92  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| P526 | K466 | D405 | E342 | A280 | K217 | E153 | N33  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| M527 | E467 | D406 | P342 | T281 | K218 | T154 | Y34  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| V528 | L468 | V407 | K343 | Y282 | E219 | D155 | R35  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| Q529 | D469 | E408 | D344 | F283 | R220 | E156 | T36  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| V530 | L470 | V409 | Y345 | L284 | A221 | E157 | L37  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| D531 | E471 | P285 | R346 | S410 | F98  | V158 | K38  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| G532 | A472 | T411 | G222 | V286 | L223 | R159 | P39  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| G533 | L473 | G412 | Q348 | G287 | R224 | E160 | E40  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| R534 | E474 | D413 | P349 | N288 | L225 | L161 | A10  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| F535 | K475 | R414 | H550 | T289 | P226 | R162 | D42  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| A536 | E476 | V415 | P351 | P290 | L227 | V163 | G43  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| T537 | L477 | A416 | N352 | L291 | F104 | G164 | L44  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| S538 | L478 | P417 | V353 | V292 | V230 | K165 | F45  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| D539 | E479 | G418 | V354 | V293 | V231 | Q166 | D46  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| L540 | E480 |      | V355 | H294 | E232 | E167 | E47  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| N541 | M481 | L421 | P356 | G295 | R233 | T168 | R48  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| D542 | K482 | A422 | E357 | G296 | E234 | V169 | A48  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| L543 | H483 | D423 | D423 | E235 | E234 | P170 | I49  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| F544 | P484 | G424 | A359 | G424 | Y236 | L171 | G51  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| R545 | S485 | G425 | R360 | E299 | K237 | P172 | P52  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| L546 | R486 | K426 | V361 | K300 | P238 | G113 | R53  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| L547 | A487 | V427 |      | G301 | T238 | V175 | R54  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| L548 | R488 | K428 | D365 | G302 | T241 | G176 | D55  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| N549 | R489 | S429 | K366 | P303 | L242 | A177 | V56  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| R550 | A490 | D430 | L243 | L304 | E243 | L178 | C57  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| N551 | K491 | V431 | V367 | A305 | E244 | K178 | E58  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| L552 | N552 | A492 | A369 | L305 | L245 | D181 | A59  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| R553 | R492 | C432 | A432 | E306 | T246 | G182 | C60  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |

|       |       |       |       |       |       |       |      |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|
| A1494 | W1434 | V1372 | L1236 | L1173 | P1048 | E987  | F919 | D859 | K799 | J737 | R675 |
| I1495 | L1435 | R1373 | I1237 | L1174 | S1049 | R988  | L920 | L860 | K800 | A738 | M676 |
| E1496 | M1238 | Q1374 | R1239 | T1115 | G1050 | R989  | R921 | Q861 | G801 | D739 | L677 |
| A1497 | A1437 | M1375 | R1239 | T1116 | G1051 | D990  | L922 | D662 | A802 | F740 | E678 |
| A1498 | A1376 | V1313 | G1245 | Y1117 | T1052 | Q991  | M924 | V863 | G803 | D742 | R679 |
| A1499 | A1339 | K1377 | V1246 | L1118 | F1053 | I992  | L924 | V864 | L804 | G743 | Q680 |
| K1500 | F1440 | V1378 | V1246 | S1119 | E1054 | L993  | E925 | T865 | E805 | D743 | R681 |
| A1501 | Q1441 | V1379 | G1316 | V1120 | E1055 | Q994  | K926 | V866 | F806 | D744 | D682 |
| E1502 | M1442 | V1380 | A1249 | V1121 | P1056 | I995  | T927 | R867 | A807 | M745 | I683 |
| E1503 | T1443 | V1381 | I1252 | L1122 | R1057 | V996  | A928 | V868 | T808 | V746 | K684 |
| A1504 | T1444 | V1382 | Q1254 | L1123 | V1058 | R997  | R123 | R869 | R909 | V747 | D685 |
| A1505 | H1445 | D1383 | Q1254 | Q1124 | S1059 | E998  | L930 | G870 | E810 | H748 | E686 |
| LVS   | V1446 | D1384 | Q1255 | E1185 | S1060 | T999  | L931 | K871 | E811 | V749 | V687 |
| GLU   | L1447 | P1387 | G1255 | V1186 | F1061 | T1000 | D932 | R872 | A812 | F750 | V688 |
| ARG   | L1448 | S1387 | L1256 | P1187 | R1062 | E1001 | A933 | L873 | L813 | L751 | D689 |
| PRO   | E1449 | R1388 | P1257 | V1188 | E974  | K1002 | L934 | K102 | A914 | S752 | A690 |
| ALA   | A1450 | L1389 | P1257 | R1189 | K935  | V936  | K935 | T875 | A815 | F753 | L691 |
| ALA   | A1451 | L1390 | V1259 | S1190 | T1066 | A1006 | Y937 | S876 | R816 | S754 | E692 |
| ARG   | T1452 | E1391 | I1260 | P1191 | V1067 | V1007 | Y937 | P877 | E817 | A755 | E693 |
| ARG   | A1453 | G1392 | E1261 | L1192 | L1068 | F1007 | G988 | Q878 | R818 | Q756 | V694 |
| GLY   | G1454 | P1392 | L1262 | T1193 | E1069 | F1008 | P989 | R879 | G819 | A757 | I695 |
| VAL   | K1455 | V1394 | F1263 | L1194 | F1070 | K1009 | T940 | R880 | E820 | E758 | H696 |
| LVS   | K1456 | L1395 | E1264 | R1195 | F1071 | M1010 | F941 | L881 | V821 | A759 | G697 |
| ARG   | D1457 | E1396 | L1335 | K1196 | I1072 | F1011 | S942 | R882 | A822 | R760 | K698 |
| GLU   | K1397 | R1197 | K1269 | R1197 | S1073 | E1012 | T943 | A883 | L823 | I761 | V699 |
| GLN   | L1458 | V1397 | A1270 | A1198 | S1074 | E1013 | T944 | R884 | N824 | V700 | V700 |
| PRO   | L1459 | D1399 | I1274 | D1199 | H1075 | M1014 | S945 | A825 | A825 | L764 | L701 |
| GLY   | G1460 | V1400 | I1277 | L1140 | G1076 | V1015 | G946 | V886 | P826 | S765 | L702 |
| LVS   | L1461 | E1401 | I1277 | A1141 | A1077 | P1016 | R947 | A887 | I827 | A766 | R703 |
| GLN   | K1462 | A1402 | C1204 | A1142 | R1078 | T948  | T948 | E888 | K828 | H767 | R704 |
| E1463 | E1464 | A1403 | G1143 | G1143 | K1079 | I949  | I949 | A889 | V829 | V768 | A705 |
| N1465 | N1465 | N1404 | G1278 | L1144 | G1080 | P1019 | Q950 | V890 | A830 | L769 | P706 |
| V1466 | I1467 | E1405 | G1279 | L1145 | G1081 | P1019 | I951 | E891 | G831 | L770 | T707 |
| I1467 | L1468 | R1406 | V1280 | Y1146 | A1082 | Y1021 | D952 | D892 | R832 | S771 | H709 |
| L1468 | L1468 | L1407 | R1281 | R1147 | D1083 | Y1022 | D953 | E893 | E833 | P772 | R709 |
| G1469 | G1469 | I1408 | I1283 | V1148 | T1084 | M1023 | K894 | T834 | T834 | A773 | R710 |
| R1470 | R1470 | A1409 | E1284 | L1149 | A1085 | A1024 | V955 | V895 | S835 | S774 | L711 |
| L1471 | L1471 | E1410 | E1285 | A1150 | L1086 | Q1025 | I956 | A896 | V836 | G775 | G712 |
| T1472 | T1472 | G1411 | T1286 | R1151 | R1087 | S1026 | P957 | W897 | G837 | E776 | I713 |
| P1473 | P1473 | K1412 | P1214 | E1152 | T1088 | G1027 | E958 | E898 | R838 | P777 | Q714 |
| A1474 | A1474 | T1413 | V1215 | V1153 | A1089 | A1028 | E959 | L899 | L839 | L778 | A715 |
| G1475 | G1475 | P1414 | Q1353 | E1154 | D1090 | R1029 | K960 | I900 | K840 | A779 | F716 |
| T1476 | T1476 | V1415 | I1217 | V1155 | S1091 | G1030 | K961 | Q901 | Y841 | K780 | Q717 |
| G1477 | G1477 | A1416 | G1218 | L1156 | G1092 | M1031 | Q962 | L902 | V842 | P781 | L720 |
| S1478 | S1478 | V1417 | E1219 | G1157 | Y1093 | P1032 | Y963 | D903 | F843 | S782 | V721 |
| D1479 | D1479 | K1418 | A1220 | V1158 | L1094 | Q1033 | L964 | V904 | N845 | D783 | Q724 |
| F1480 | F1480 | P1419 | V1221 | R1159 | T1095 | Q1034 | E965 | P905 | N845 | D784 | S725 |
| V1481 | V1481 | L1420 | E1295 | L1160 | R1096 | I1035 | E966 | Q906 | P846 | I785 | I726 |
| R1482 | R1482 | L1421 | S1296 | E1161 | K1097 | R1036 | A967 | E907 | D847 | I786 | I726 |
| F1483 | F1483 | M1422 | E1297 | E1162 | L1098 | Q1037 | D968 | K908 | E848 | L787 | I726 |
| T1484 | T1484 | G1423 | G1298 | G1163 | V1099 | L1038 | R969 | N909 | A849 | G788 | Q727 |
| Q1485 | Q1485 | V1424 | F1299 | R1164 | D1100 | C1039 | K970 | S910 | L850 | L728 | L728 |
| V1486 | V1486 | T1425 | S1300 | Y1165 | V1101 | G1040 | L971 | L911 | L851 | H729 | H729 |
| K1487 | K1487 | K1426 | K1301 | L1166 | T1102 | L1041 | L972 | K912 | A852 | I792 | P730 |
| D1488 | D1488 | A1427 | E1302 | S1167 | L1167 | K1042 | Q973 | R953 | R853 | T793 | L731 |
| O1489 | O1489 | A1428 | E1303 | M1168 | E1103 | G1043 | L983 | V915 | E855 | V795 | C733 |
| K1490 | K1490 | L1429 | K1304 | D1169 | L1105 | L1044 | L983 | V916 | G856 | V796 | E734 |
| T1491 | T1491 | S1430 | K1304 | D1170 | V1106 | M1045 | T984 | Y916 | Q856 | R796 | E734 |
| L1492 | L1492 | P1431 | L1305 | V1171 | V1107 | Q1046 | D985 | Q917 | K157 | K797 | A735 |
| K1493 | K1493 | V1371 | P1306 | H1172 | R1108 | K1047 | R986 | A918 | V858 | E798 | F736 |

• Molecule 3: BACTERIAL RNA POLYMERASE BETA-PRIME SUBUNIT; CHAIN D, N

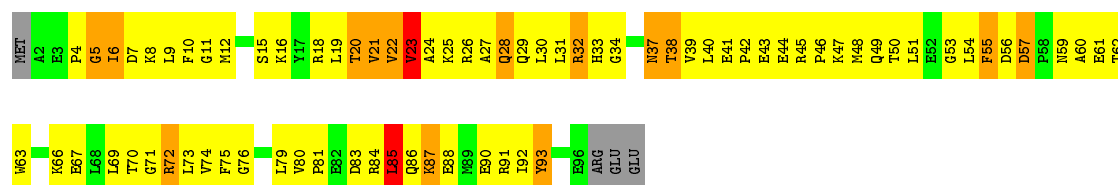


|       |       |      |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|
| T997  | L930  | Y868 | T808 | A746 | Q616 | K555 | R495 | V435 | A370 | G309 | P248 | V186 | K64  |
| E996  | L931  | K871 | P809 | V747 | M617 | K556 | L496 | E436 | L371 | L310 | Y249 | K187 | R65  |
| T999  | D932  | K872 | E811 | V748 | L618 | L557 | E497 | V437 | B372 | L311 | L250 | G188 | Q66  |
| T1000 | A933  | R873 | E812 | V749 | L619 | L558 | V498 | D438 | P373 | R312 | F251 | P189 | Y128 |
| E1001 | L934  | L873 | A813 | P750 |      | A559 | R500 | L439 | E374 | R313 | R252 | E190 | F129 |
| K1002 | K935  | E874 | L813 | P751 |      | Q560 | R501 | V440 | E375 | P314 | A253 | L191 | G70  |
| Y1003 | Y836  | T875 | A814 |      | R622 | G561 | A501 | R441 | E376 | R315 | E254 | K131 | K71  |
| T1004 | Y837  | S876 | A815 | F754 | V623 | A562 | F502 | M442 | P377 | Q316 | E255 | Y132 | V72  |
| Q1005 | G938  | R877 | R816 | A755 | D624 | P663 | L503 | V443 | L378 | V317 | E256 | I133 | C73  |
| A1006 | P939  | G878 | R817 | A756 | S626 | E564 | D504 | R444 | A379 | R318 | G257 | V134 | E74  |
| V1007 | T940  | R879 | R818 | A757 | G627 | I565 | S505 | V445 | E380 | A319 | V258 | L135 | R75  |
| F1008 | F941  | I880 | G819 | E758 | R628 | I566 | G506 | V446 | A381 | A320 | V259 | D136 | C76  |
| K1009 | S942  | L881 | E820 | A759 | G629 | I567 | N507 | V447 |      | Q321 | E260 | P137 | G77  |
| H1010 | T943  | F882 | V821 | R760 | V630 | R568 | R508 | E448 |      | V322 | L261 | L199 | G77  |
| F1011 | T944  | A883 | A822 | I761 | L631 | N569 | P509 | E448 | V385 | E329 | L262 | D200 | V78  |
| N1012 | S945  | L884 | L823 | Q762 | V632 | E570 | E510 | Y450 | L387 | E323 | R263 | G201 | E79  |
| E1013 | G946  | I885 | N824 | N763 | G633 | K571 | N511 | D451 | R388 | A324 | E263 | V202 | V80  |
| H1014 | I947  | V886 | A825 | L764 | G634 | R572 | N512 | I452 | R389 | E325 | L264 | A203 | T81  |
| Y1015 | T948  | A887 | R826 | S765 | P635 | R573 | L513 | D453 | E389 | E326 | E265 | L204 | T82  |
| P1016 | I949  | E888 | I827 | A766 | Q636 | L574 | L514 | A454 | P390 | E327 | E266 | Y205 | S83  |
| F1017 | G950  | A889 | K828 | H767 | L637 | Q575 | E515 | A454 | A391 | G328 | G267 | R206 | I84  |
| N1018 | V890  | V890 | V829 | A773 | K638 | E576 | A516 | N456 | S392 | E329 | A268 | P207 | V85  |
| P1019 | D952  | E891 | A830 | L769 | L639 | A577 | V517 | Q457 | L394 | V330 | F269 | P208 | R86  |
| L1020 | D953  | D892 | G831 | L770 | H640 | N578 | P518 | A458 | L394 | V332 | L270 | R209 | R87  |
| Y1021 | A954  | E893 | R832 | S771 | N703 | D579 | V519 | E459 | V396 | L333 | L272 | R210 | Y88  |
| V1022 | V855  | K894 | E833 | P772 | R704 | A580 | L520 | A460 | K397 | T334 | R273 | R212 | R89  |
| M1023 | I956  | A895 | T834 | A773 |      | L581 | P521 | I461 | A398 | L335 | R274 | E213 | M90  |
| A1024 | S957  | A896 | S835 | S774 |      | L582 | P522 | Q462 | R399 | E336 | E275 | V214 | G91  |
| Q1025 | E958  | V897 | V836 | G775 |      | D583 | N524 | Q463 | V400 | L337 | D276 | E215 | R92  |
| S1026 | E959  | E998 | G837 |      |      | N584 | L524 | L464 | Y401 | E338 | E277 | V216 | I93  |
| G1027 | K960  | L899 | R838 | L778 |      | G585 | R525 | L465 | P402 | V339 | P278 | K217 | E94  |
| A1028 | K961  | I900 | L839 | A779 |      | R586 | P526 | K466 | P403 | T340 | V279 | K218 | L95  |
| R1029 | Q940  | Q901 | R840 | K780 |      | R587 | N527 | K467 | E404 | E341 | A280 | E219 | A86  |
| G1030 | L963  | L902 | Y841 | P781 |      | P590 | V528 | L468 | D406 | P342 | T281 | R220 | T97  |
| M1031 | L964  | P904 | F943 | R783 |      | V591 | V530 | L470 | V407 | E282 | Y282 | A221 | P88  |
| P1032 | E965  | P905 | A844 | D784 |      | T592 | D531 | E471 | E408 | F283 | G222 | L223 | A100 |
| Q1033 | E966  | Q906 | N845 | I785 |      | N593 | G533 | A472 | V409 | L284 | L223 | L224 | H101 |
| I1034 | A967  | Q907 | P846 | I786 |      | P594 | R534 | L473 | S410 | P285 | E225 | L225 | I102 |
| R1036 | D968  | K908 | D847 | L787 |      | G595 | F535 | E474 | T411 | G286 | P226 | L226 | M103 |
| Q1037 | K970  | N909 | E848 | G788 |      | S596 | A536 | K475 | Q412 | Q348 | G287 | L227 | F104 |
| L1038 | L971  | S910 | A949 | L789 |      | D597 | L658 | E476 | D413 | R350 | T288 | L227 | V105 |
| C1039 | L972  | L911 | L850 | V790 |      | R598 | T537 | L477 | R414 | K352 | T289 | A228 | K106 |
| G1040 | Q973  | K912 | L851 | Y791 |      | P599 | N538 | L478 | V415 | V353 | P290 | A229 | D107 |
| L1041 | I974  |      | A852 | I792 |      | L600 | D539 | E479 | A416 | V354 | L281 | W230 | V108 |
| G1043 |       | V915 | V853 | I793 |      | R601 | L540 | E480 | P417 | V355 | V282 | K233 | P109 |
|       | L983  | Y916 | A854 | Q794 |      | S602 | N541 | N481 | Q418 | P356 | H294 | E234 | S110 |
|       | T984  | Q117 | R855 | V795 |      | L603 | D542 | K482 | D419 | E357 | G295 | A235 | I112 |
|       | D985  | A918 | G856 | R796 |      | T604 | L543 | H483 | V420 | G358 | E296 | Y236 | G113 |
|       | R986  | F919 | I857 | K797 |      | D605 | V544 | P484 | L421 | A359 | L297 | K237 | T114 |
| P1048 | E987  | L820 | V858 | E798 |      | A667 | R545 | S488 | A422 | K360 | V298 | P238 | L115 |
| S1049 | R988  | R921 | D859 | K799 |      | P668 | R546 | R486 | D423 | V361 | E299 | G239 | D176 |
| G1050 | Y989  | L922 | L860 | N737 |      | M669 | S608 | A487 |      | K300 | E240 | K239 | D117 |
| E1051 | D990  | G923 | Q861 | A738 |      | G609 | L548 | R488 | K428 | A363 | L241 | I241 | L118 |
| T1052 | Q991  | M924 | D862 | F739 |      | K610 | N549 | R489 | S429 | G364 | Q302 | L242 | S119 |
| F1053 |       | E925 | V863 | F740 |      | Q611 | R550 | A490 | D430 | D365 | A243 | K180 | A120 |
|       | L993  | K926 | V864 | A673 |      | G612 | N551 | K491 | V431 | K366 | E244 | E244 | T121 |
|       | Q994  | T927 | T865 | R674 |      | R613 | N552 | A492 | Y432 | L367 | L245 | P246 | E122 |
| P1056 | V1057 | F066 | V866 | Q744 |      | G614 | R553 | R493 | G433 | V368 | A307 | P246 | L123 |
|       | R1058 | W996 | R867 | M745 |      | R615 | L554 | K494 | R434 | A369 | K308 | E247 | E183 |



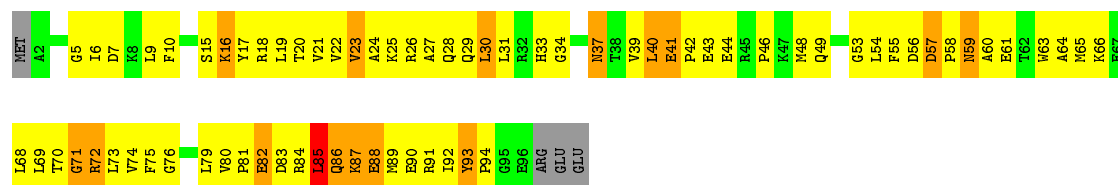
• Molecule 4: BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O

Chain E: 19% 61% 14%



• Molecule 4: BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O

Chain O: 23% 57% 15%



• Molecule 5: RNA polymerase principal sigma factor (RpoD); CHAIN F, P

Chain F: 9% 57% 16% 17%



|     |     |      |      |      |      |      |      |      |      |      |      |      |
|-----|-----|------|------|------|------|------|------|------|------|------|------|------|
| LYS | ASP | G121 | A182 | Q245 | L308 | V368 | L369 | L309 | Q246 | A183 | L308 | V368 |
| LYS | LEU | L122 | A183 | A246 | K309 | L369 | K370 | K309 | A247 | L123 | K309 | L369 |
| GLU | LEU | D123 | Q185 | M248 | A311 | K371 | A311 | A311 | M249 | D124 | A311 | K371 |
| SER | GLU | P124 | H186 | L251 | Q312 | K372 | K372 | Q312 | L252 | P125 | Q312 | K372 |
| LYS | GLU | D125 | L187 | L252 | E313 | K373 | K373 | E313 | L253 | D126 | E313 | K373 |
| ARG | LYS | L126 | L188 | L253 | E314 | G374 | G374 | E314 | L254 | L127 | E314 | G374 |
| LYS | ASN | L127 | L189 | L254 | S315 | L375 | L375 | S315 | L255 | L128 | S315 | L375 |
| ALA | ASP | R128 | E189 | A255 | S316 | L376 | L376 | S316 | A256 | R129 | S316 | L376 |
| GLN | LEU | E129 | A190 | R256 | S317 | D377 | D377 | S317 | R257 | E130 | S317 | D377 |
| ALA | PRQ | V130 | N191 | T257 | E318 | G378 | G378 | E318 | T258 | V131 | E318 | G378 |
| ALA | PRQ | V131 | L192 | L258 | E319 | R379 | R379 | E319 | L259 | R132 | E319 | R379 |
| ILE | GLN | R132 | R193 | R259 | T319 | R379 | R379 | T319 | R260 | R133 | T319 | R379 |
| GLU | PRQ | A133 | L194 | L260 | P320 | E380 | E380 | P320 | L261 | A134 | P320 | E380 |
| ALA | ALA | K134 | V195 | P261 | I321 | H381 | H381 | I321 | P262 | K135 | I321 | H381 |
| GLN | GLN | L135 | V196 | E262 | G322 | T382 | T382 | G322 | E263 | L136 | G322 | T382 |
| GLN | THR | S76  | S197 | H263 | D323 | L383 | L383 | D323 | H264 | S77  | D323 | L383 |
| THR | THR | G137 | I198 | V264 | E324 | E384 | E384 | E324 | V265 | G138 | E324 | E384 |
| GLU | GLU | S138 | L265 | E266 | K325 | E385 | E385 | K325 | E267 | S139 | E385 | E385 |
| VAL | VAL | A139 | T203 | E268 | D326 | G386 | G386 | D326 | T269 | A140 | G386 | G386 |
| LEU | LEU | R140 | G204 | T267 | S327 | V387 | V387 | S327 | T270 | R141 | V387 | V387 |
| VAL | VAL | V81  | R205 | T268 | F328 | A388 | A388 | F328 | T269 | V82  | A388 | A388 |
| GLN | GLN | R82  | G206 | M269 | Y329 | V392 | V392 | Y329 | M270 | R83  | V392 | V392 |
| GLU | GLU | Q83  | L207 | K270 | G330 | T393 | T393 | G330 | L271 | Q84  | T393 | T393 |
| GLU | GLU | H84  | S208 | L271 | D331 | R394 | R394 | D331 | L272 | H85  | R394 | R394 |
| ALA | ALA | P145 | F209 | S272 | E332 | E395 | E395 | E332 | S273 | P146 | E395 | E395 |
| GLU | GLU | G146 | L210 | R273 | I333 | R396 | R396 | I333 | L211 | G147 | R396 | R396 |
| GLU | GLU | E87  | D211 | T274 | P334 | A400 | A400 | P334 | T275 | E88  | A400 | A400 |
| PRQ | PRQ | K148 | L212 | A275 | D335 | L401 | L401 | D335 | A276 | K149 | L401 | L401 |
| LEU | LEU | G89  | T213 | R276 | E336 | Q399 | Q399 | E336 | T277 | G90  | Q399 | Q399 |
| GLU | GLU | Q90  | Q214 | Q277 | H337 | R399 | R399 | H337 | Q278 | Q91  | R399 | R399 |
| PHE | PHE | L151 | E215 | L278 | I338 | I400 | I400 | I338 | L279 | L152 | I400 | I400 |
| PRQ | PRQ | D152 | G216 | Q279 | P339 | E401 | E401 | P339 | Q280 | D153 | E401 | E401 |
| GLU | GLU | P153 | N217 | Q280 | S340 | N402 | N402 | S340 | E281 | P154 | N402 | N402 |
| GLY | GLY | K154 | Q218 | E281 | F341 | A404 | A404 | F341 | L282 | K155 | A404 | A404 |
| PRQ | PRQ | T155 | G219 | L282 | V342 | L405 | L405 | V342 | G283 | T156 | L405 | L405 |
| ASP | ASP | V156 | L220 | G283 | D343 | R406 | R406 | D343 | E284 | V157 | R406 | R406 |
| LEU | LEU | E97  | L221 | R284 | A344 | K407 | K407 | A344 | E285 | E98  | K407 | K407 |
| GLU | GLU | E98  | R222 | E285 | A345 | L408 | L408 | A345 | T286 | E99  | L408 | L408 |
| ASP | ASP | E99  | A223 | T287 | T346 | K409 | K409 | T346 | T288 | E101 | K409 | K409 |
| LEU | LEU | V100 | D160 | T287 | Q347 | H410 | H410 | Q347 | Y288 | E102 | H410 | H410 |
| ASP | ASP | E101 | Q161 | E288 | S348 | H411 | H411 | S348 | E289 | E103 | H411 | H411 |
| GLU | GLU | L102 | K162 | E289 | L349 | E412 | E412 | L349 | E290 | L103 | E412 | E412 |
| PRQ | PRQ | A103 | L163 | E290 | L350 | S413 | S413 | L350 | E291 | A104 | S413 | S413 |
| ASP | ASP | R104 | K164 | E291 | S351 | R414 | R414 | S351 | A292 | R105 | R414 | R414 |
| LEU | LEU | K105 | S165 | A292 | E352 | T415 | T415 | E352 | E293 | K106 | T415 | T415 |
| THR | THR | V106 | L166 | E293 | E353 | R417 | R417 | E353 | A294 | V107 | R417 | R417 |
| GLU | GLU | E107 | P167 | E294 | L354 | K417 | K417 | L354 | E295 | E108 | K417 | K417 |
| ASP | ASP | G109 | R231 | M295 | E355 | L418 | L418 | E355 | G296 | G110 | L418 | L418 |
| ASP | ASP | G109 | R232 | G296 | K356 | R419 | R419 | K356 | P297 | G111 | R419 | R419 |
| LEU | LEU | M110 | H170 | P297 | A357 | D420 | D420 | A357 | G298 | E111 | D420 | D420 |
| LEU | LEU | E111 | K171 | G298 | L358 | F421 | F421 | L358 | E299 | E112 | F421 | F421 |
| ASP | ASP | A112 | R172 | E299 | S359 | L422 | L422 | S359 | M299 | A113 | L422 | L422 |
| LEU | LEU | I113 | Y173 | D300 | K360 | A301 | A301 | K360 | D301 | I114 | A301 | A301 |
| PRQ | PRQ | K114 | Y173 | A301 | L361 | S362 | S362 | L361 | K302 | K115 | S362 | S362 |
| GLU | GLU | L115 | H175 | K302 | E363 | R303 | R303 | E363 | L116 | L116 | R303 | R303 |
| GLU | GLU | L116 | I176 | R303 | R364 | E365 | E365 | R364 | I177 | L117 | E365 | E365 |
| GLY | GLY | S117 | A177 | R304 | E366 | E366 | E366 | E366 | A178 | S118 | E366 | E366 |
| GLY | GLY | E118 | R178 | E306 | M367 | M367 | M367 | M367 | E119 | E119 | M367 | M367 |
| GLY | GLY | I119 | L243 | E306 | M367 | M367 | M367 | M367 | L244 | I120 | M367 | M367 |
| GLY | GLY | T120 | E181 | T307 | M367 | M367 | M367 | M367 | E181 | T120 | M367 | M367 |

• Molecule 5: RNA polymerase principal sigma factor (RpoD); CHAIN F, P

Chain P: 9% 55% 18% 17%

|      |      |      |      |      |      |     |
|------|------|------|------|------|------|-----|
| E365 | R303 | T243 | E181 | G121 | LEU  | MET |
| R304 | R303 | R244 | A182 | L122 | ASP  | LYS |
| E366 | E305 | Q245 | A183 | D123 | LEU  | LYS |
| V368 | E306 | A246 | R184 | P124 | GLU  | SER |
| L369 | T307 | T247 | Q185 | D125 | GLU  | LYS |
| K370 | L308 | N248 | H186 | L126 | GLU  | ARG |
| K309 | K309 | R249 | L187 | L127 | GLU  | LYS |
| R372 | I310 | A250 | E188 | R128 | GLU  | ASN |
| K373 | K311 | T251 | E189 | E129 | ASP  | ALA |
| G374 | Q312 | A252 | A190 | V130 | LEU  | GLN |
| E313 | E313 | D253 | N191 | V131 | PRQ  | ALA |
| I376 | P314 | Q254 | L192 | R132 | ILE  | GLN |
| D377 | V315 | A255 | R193 | A133 | PRQ  | GLU |
| G378 | S316 | R256 | L194 | K134 | K74  | ALA |
| R379 | L317 | T257 | V195 | L135 | R75  | GLN |
| E380 | E318 | L258 | V196 | L136 | S76  | GLU |
| H381 | T319 | R259 |      | G137 | T77  | THR |
| E382 | P320 | L260 | K200 | S138 | S78  | GLU |
| L383 | I321 | P261 | K201 | A139 | D79  | VAL |
| E384 | G322 | V262 | T202 | R140 | P80  | LEU |
| E385 | D323 | H263 | T203 | V141 | V81  | VAL |
| V386 | E324 | M264 | G204 | R142 | R82  | GLN |
| G387 | K325 | V265 | R205 | H143 | O83  | GLU |
| E388 | D326 | E266 | G206 | I144 | H84  | GLU |
| F389 | S327 | T267 | L207 | P145 | L85  | ALA |
| V392 | F328 | L268 | S208 | G146 | H86  | GLU |
| R393 | Y329 | N269 | F209 | L147 | E87  | GLU |
| R394 | G330 | K270 | L210 | K148 | I88  | LEU |
| R395 | F332 | L271 | D211 | E149 | G89  | PRQ |
| R396 | R333 | S272 | L212 | T150 | Q90  | GLU |
| L397 | P334 | R273 | I213 | L151 | V91  | PHE |
| R398 | R335 | T274 | Q214 | D152 | P92  | PRQ |
| Q399 | E336 | G276 | E215 | P153 | P93  | GLU |
| L400 |      | R275 | G216 | K154 | L94  | GLY |
| E401 | P339 | Q277 | N217 | T155 | T95  | GLU |
| N402 |      | L278 | Q218 | V156 | L96  | PRQ |
| K403 | V342 | Q279 | G219 | E157 | E97  | ASP |
| A404 | D343 | R280 | L220 | E158 | E98  | PRQ |
| L405 | A344 | E281 | I221 | I159 | E99  | ASP |
| R406 | A345 | L282 | R222 | D160 | LEU  | LEU |
| K407 | T346 | G283 | A223 | Q161 | E101 | GLU |
| L408 | Q347 | R284 | V224 | K162 | L102 | ASP |
| K409 | S348 | E285 | E225 | L163 | A103 | PRQ |
| Y410 | L349 | P286 | K226 | K164 | R104 | ASP |
| H411 | L350 | T287 | F227 | S165 | K105 | LEU |
| E412 | S351 | Y288 | E228 | L166 | V106 | THR |
| S413 | E352 | E289 | Y229 | P167 | E107 | LEU |
| R414 | E353 | E290 | K230 | K168 | E108 | GLU |
| L416 | L354 | A292 | R231 | E169 | G109 | ASP |
| K417 | E355 | E293 | F233 | H170 | M110 | ASP |
| L418 | A356 | A294 | K234 | K171 | E111 | LEU |
| R419 | L358 | M295 | F235 | R172 | A112 | ASP |
| F421 | S359 | G296 | E236 | Y173 | I113 | LEU |
| L422 | K360 | P297 | T237 | L174 | K114 | PRQ |
| ASP  | L361 | Q299 | Y238 | H175 | K115 | GLU |
|      | S362 | R300 | A239 | A177 | E117 | GLY |
|      | E363 | A301 | T240 | R178 | A118 | GLY |
|      | R364 | E302 | W241 | E179 | I119 | GLY |
|      |      | E302 | W242 | C180 | F186 | GLY |

## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 32   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 235.09 Å   235.09 Å   250.88 Å<br>90.00°   90.00°   120.00°    | Depositor        |
| Resolution (Å)  | 50.00 – 3.00<br>46.80 – 3.00                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.3 (50.00-3.00)<br>96.0 (46.80-3.00)                         | Depositor<br>EDS |
| $R_{merge}$   | 0.11   | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.52 (at 3.01 Å)   | Xtriage          |
| Refinement program  | CNS  | Depositor        |
| R, $R_{free}$   | 0.235   ,   0.289<br>0.221   ,   0.274                         | Depositor<br>DCC |
| $R_{free}$ test set   | 2351 reflections (0.79%)                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 83.8   | Xtriage          |
| Anisotropy  | 0.053  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.25   ,   46.6  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$    | Xtriage          |
| Estimated twinning fraction   | 0.499 for -h,-k,l<br>0.047 for h,-h-k,-l<br>0.047 for -k,-h,-l | Xtriage          |
| $F_o, F_c$ correlation  | 0.95   | EDS              |
| Total number of atoms   | 56149  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 81.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN, MPD, NE6, MG

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.43         | 0/1848         | 0.73        | 0/2512          |
| 1   | B     | 0.39         | 0/1936         | 0.68        | 0/2633          |
| 1   | K     | 0.43         | 0/1848         | 0.72        | 1/2512 (0.0%)   |
| 1   | L     | 0.41         | 0/1936         | 0.70        | 0/2633          |
| 2   | C     | 0.43         | 0/8997         | 0.73        | 8/12164 (0.1%)  |
| 2   | M     | 0.43         | 0/8997         | 0.73        | 3/12164 (0.0%)  |
| 3   | D     | 0.44         | 0/12073        | 0.77        | 11/16324 (0.1%) |
| 3   | N     | 0.46         | 2/12073 (0.0%) | 0.76        | 9/16324 (0.1%)  |
| 4   | E     | 0.40         | 0/783          | 0.69        | 0/1054          |
| 4   | O     | 0.41         | 0/783          | 0.65        | 0/1054          |
| 5   | F     | 0.40         | 0/2874         | 0.72        | 1/3866 (0.0%)   |
| 5   | P     | 0.40         | 0/2874         | 0.69        | 1/3866 (0.0%)   |
| All | All   | 0.43         | 2/57022 (0.0%) | 0.74        | 34/77106 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | N     | 0                   | 1                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | N     | 58  | CYS  | CB-SG | -5.87 | 1.72        | 1.81     |
| 3   | N     | 60  | CYS  | CB-SG | -5.42 | 1.73        | 1.81     |

All (34) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 3   | D     | 831  | GLY  | N-CA-C   | -12.95 | 80.74       | 113.10   |
| 3   | N     | 831  | GLY  | N-CA-C   | -11.03 | 85.51       | 113.10   |
| 2   | C     | 177  | GLU  | N-CA-C   | -8.93  | 86.88       | 111.00   |
| 5   | F     | 313  | GLU  | N-CA-C   | 8.15   | 133.01      | 111.00   |
| 2   | M     | 58   | ASP  | N-CA-C   | -8.08  | 89.18       | 111.00   |
| 3   | D     | 803  | GLY  | N-CA-C   | -7.75  | 93.74       | 113.10   |
| 2   | M     | 177  | GLU  | N-CA-C   | -7.54  | 90.65       | 111.00   |
| 3   | N     | 803  | GLY  | N-CA-C   | -7.53  | 94.27       | 113.10   |
| 5   | P     | 313  | GLU  | N-CA-C   | 7.14   | 130.27      | 111.00   |
| 2   | C     | 58   | ASP  | N-CA-C   | -6.66  | 93.03       | 111.00   |
| 3   | D     | 1128 | VAL  | N-CA-C   | -6.34  | 93.87       | 111.00   |
| 2   | C     | 177  | GLU  | C-N-CD   | -6.19  | 106.98      | 120.60   |
| 3   | D     | 798  | GLU  | N-CA-C   | 6.16   | 127.63      | 111.00   |
| 3   | N     | 1128 | VAL  | N-CA-C   | -6.03  | 94.72       | 111.00   |
| 3   | D     | 799  | LYS  | N-CA-C   | 5.89   | 126.90      | 111.00   |
| 3   | N     | 1125 | PRO  | N-CA-C   | 5.87   | 127.37      | 112.10   |
| 3   | N     | 199  | LEU  | CA-CB-CG | -5.65  | 102.30      | 115.30   |
| 3   | D     | 131  | LYS  | N-CA-C   | 5.54   | 125.95      | 111.00   |
| 3   | N     | 799  | LYS  | N-CA-C   | 5.35   | 125.44      | 111.00   |
| 2   | C     | 182  | VAL  | N-CA-C   | -5.29  | 96.72       | 111.00   |
| 3   | D     | 807  | ALA  | N-CA-C   | -5.28  | 96.74       | 111.00   |
| 2   | M     | 1092 | LEU  | CA-CB-CG | -5.27  | 103.19      | 115.30   |
| 3   | D     | 410  | SER  | N-CA-C   | 5.23   | 125.13      | 111.00   |
| 3   | N     | 798  | GLU  | N-CA-C   | 5.20   | 125.04      | 111.00   |
| 3   | N     | 807  | ALA  | N-CA-C   | -5.19  | 96.99       | 111.00   |
| 3   | D     | 830  | ALA  | N-CA-C   | 5.17   | 124.96      | 111.00   |
| 2   | C     | 675  | ALA  | N-CA-C   | -5.10  | 97.23       | 111.00   |
| 3   | N     | 144  | GLY  | N-CA-C   | -5.09  | 100.37      | 113.10   |
| 2   | C     | 165  | LEU  | N-CA-C   | 5.08   | 124.72      | 111.00   |
| 2   | C     | 178  | PRO  | N-CA-C   | 5.06   | 125.26      | 112.10   |
| 3   | D     | 717  | GLN  | N-CA-C   | -5.06  | 97.35       | 111.00   |
| 1   | K     | 47   | SER  | N-CA-C   | 5.03   | 124.57      | 111.00   |
| 2   | C     | 9    | ILE  | N-CA-C   | -5.02  | 97.44       | 111.00   |
| 3   | D     | 1286 | THR  | N-CA-C   | -5.00  | 97.50       | 111.00   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 3   | N     | 1117 | TYR  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1816  | 0        | 1871     | 279     | 0            |
| 1   | B     | 1902  | 0        | 1951     | 321     | 0            |
| 1   | K     | 1816  | 0        | 1871     | 296     | 0            |
| 1   | L     | 1902  | 0        | 1951     | 318     | 0            |
| 2   | C     | 8829  | 0        | 8933     | 1694    | 0            |
| 2   | M     | 8829  | 0        | 8933     | 1598    | 0            |
| 3   | D     | 11864 | 0        | 12094    | 2489    | 0            |
| 3   | N     | 11864 | 0        | 12094    | 2441    | 0            |
| 4   | E     | 769   | 0        | 775      | 163     | 0            |
| 4   | O     | 769   | 0        | 775      | 123     | 0            |
| 5   | F     | 2829  | 0        | 2914     | 587     | 0            |
| 5   | P     | 2829  | 0        | 2914     | 671     | 0            |
| 6   | A     | 5     | 0        | 0        | 0       | 0            |
| 6   | D     | 5     | 0        | 0        | 1       | 0            |
| 7   | B     | 1     | 0        | 0        | 0       | 0            |
| 7   | D     | 1     | 0        | 0        | 0       | 0            |
| 7   | N     | 1     | 0        | 0        | 0       | 0            |
| 8   | C     | 16    | 0        | 26       | 0       | 0            |
| 8   | M     | 8     | 0        | 13       | 0       | 0            |
| 9   | D     | 2     | 0        | 0        | 0       | 0            |
| 9   | N     | 2     | 0        | 0        | 0       | 0            |
| 10  | D     | 30    | 0        | 30       | 8       | 0            |
| 10  | N     | 30    | 0        | 30       | 7       | 0            |
| 11  | A     | 1     | 0        | 0        | 1       | 0            |
| 11  | B     | 1     | 0        | 0        | 1       | 0            |
| 11  | C     | 7     | 0        | 0        | 2       | 0            |
| 11  | D     | 10    | 0        | 0        | 0       | 0            |
| 11  | F     | 1     | 0        | 0        | 1       | 0            |
| 11  | M     | 5     | 0        | 0        | 1       | 0            |
| 11  | N     | 4     | 0        | 0        | 0       | 0            |
| 11  | O     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 56149 | 0        | 57175    | 10419   | 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 92.

All (10419) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:283:ILE:HG22  | 2:M:284:ARG:H    | 1.03                     | 1.17              |
| 3:D:416:ALA:HB2   | 3:D:432:TYR:HA   | 1.19                     | 1.17              |
| 3:D:1489:GLN:HA   | 3:D:1492:LEU:HG  | 1.23                     | 1.17              |
| 3:N:272:LEU:HD12  | 3:N:280:ALA:HB3  | 1.23                     | 1.16              |
| 1:A:14:ARG:HB2    | 1:B:233:VAL:HA   | 1.27                     | 1.16              |
| 3:N:322:VAL:HA    | 3:N:335:LEU:HG   | 1.20                     | 1.16              |
| 2:C:178:PRO:O     | 2:C:220:GLY:HA2  | 1.40                     | 1.15              |
| 3:D:237:LYS:HB3   | 3:D:238:PRO:HD2  | 1.25                     | 1.15              |
| 2:M:264:PRO:HB2   | 2:M:289:THR:HG21 | 1.24                     | 1.15              |
| 3:N:416:ALA:HB2   | 3:N:432:TYR:HA   | 1.16                     | 1.15              |
| 3:D:1481:VAL:HG11 | 4:E:18:ARG:HA    | 1.18                     | 1.15              |
| 2:C:304:LEU:HB3   | 2:C:305:PRO:HD3  | 1.24                     | 1.15              |
| 3:D:297:ILE:HD13  | 3:D:298:VAL:HG23 | 1.24                     | 1.14              |
| 3:D:353:VAL:HA    | 3:D:368:VAL:HG22 | 1.17                     | 1.14              |
| 3:N:421:LEU:HG    | 3:N:428:LYS:HA   | 1.20                     | 1.14              |
| 2:C:267:TYR:HB2   | 2:C:272:ALA:HB2  | 1.25                     | 1.14              |
| 3:D:258:VAL:HB    | 3:D:273:ARG:HB2  | 1.15                     | 1.14              |
| 3:N:353:VAL:HA    | 3:N:368:VAL:HG22 | 1.22                     | 1.13              |
| 2:M:72:ARG:HG2    | 2:M:95:TYR:HB2   | 1.27                     | 1.13              |
| 3:D:249:TYR:HB3   | 3:D:307:ALA:HB3  | 1.14                     | 1.13              |
| 3:N:244:GLU:O     | 3:N:246:PRO:HD3  | 1.49                     | 1.13              |
| 3:D:931:LEU:HA    | 3:D:934:LEU:HD12 | 1.30                     | 1.12              |
| 2:C:580:MET:HB3   | 2:C:584:GLU:OE2  | 1.50                     | 1.12              |
| 5:P:418:LEU:H     | 5:P:418:LEU:HD12 | 1.08                     | 1.12              |
| 3:N:1494:ALA:HA   | 3:N:1497:GLU:HG2 | 1.16                     | 1.12              |
| 3:D:274:ARG:HB3   | 3:D:279:VAL:HG21 | 1.26                     | 1.11              |
| 1:B:137:ARG:HH12  | 1:B:139:ASN:HB2  | 1.07                     | 1.11              |
| 2:M:15:LEU:H      | 2:M:15:LEU:HD12  | 1.02                     | 1.11              |
| 3:D:368:VAL:HB    | 3:D:377:VAL:HG21 | 1.33                     | 1.11              |
| 3:D:534:ARG:NH2   | 5:F:313:GLU:HB2  | 1.66                     | 1.11              |
| 1:B:206:THR:HB    | 1:B:209:GLU:HG3  | 1.32                     | 1.10              |
| 1:L:76:VAL:HA     | 1:L:79:ILE:HD12  | 1.33                     | 1.10              |
| 2:M:150:PRO:HA    | 2:M:158:TYR:HB3  | 1.26                     | 1.10              |
| 3:D:1217:ILE:HD12 | 3:D:1217:ILE:H   | 1.15                     | 1.10              |
| 3:D:119:SER:HB3   | 3:D:123:LEU:H    | 1.13                     | 1.10              |
| 3:D:804:LEU:HB2   | 3:D:809:PRO:HG3  | 1.11                     | 1.10              |
| 3:D:188:GLY:H     | 3:D:198:ARG:HA   | 0.99                     | 1.10              |
| 3:D:582:LEU:HA    | 3:D:603:LEU:HD12 | 1.24                     | 1.10              |
| 2:C:31:GLN:HG2    | 2:C:35:PRO:HB3   | 1.25                     | 1.10              |
| 5:F:413:SER:HA    | 5:F:416:ARG:CZ   | 1.81                     | 1.09              |
| 2:C:72:ARG:HG2    | 2:C:95:TYR:HB2   | 1.31                     | 1.09              |
| 3:N:548:ILE:HG22  | 3:N:552:ASN:HD21 | 1.11                     | 1.09              |

Continued on next page...

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:34:VAL:HB     | 1:B:42:ARG:HH12   | 1.02                     | 1.09              |
| 3:D:658:LEU:HA    | 3:D:661:MET:HE3   | 1.25                     | 1.09              |
| 2:M:650:ARG:N     | 2:M:650:ARG:HE    | 1.50                     | 1.09              |
| 3:N:237:LYS:HB3   | 3:N:238:PRO:HD2   | 1.28                     | 1.09              |
| 2:C:59:LYS:HD2    | 2:C:59:LYS:H      | 1.18                     | 1.09              |
| 3:D:530:VAL:HG23  | 3:D:531:ASP:H     | 1.10                     | 1.09              |
| 2:M:230:ARG:HE    | 2:M:233:GLU:HG2   | 1.06                     | 1.09              |
| 1:A:206:THR:HB    | 1:A:209:GLU:HG3   | 1.33                     | 1.09              |
| 5:F:113:ILE:HA    | 5:F:116:LEU:HD12  | 1.35                     | 1.08              |
| 3:N:1101:VAL:HG22 | 3:N:1428:ALA:HB2  | 1.30                     | 1.08              |
| 3:N:227:LEU:HA    | 3:N:331:VAL:HG23  | 1.18                     | 1.08              |
| 2:C:115:LEU:HD11  | 2:C:373:VAL:CG1   | 1.83                     | 1.08              |
| 5:P:302:LYS:HD2   | 5:P:303:ARG:N     | 1.68                     | 1.08              |
| 2:M:192:PRO:O     | 2:M:195:LEU:HG    | 1.53                     | 1.08              |
| 3:N:148:GLU:HB3   | 3:N:151:GLN:HB2   | 1.34                     | 1.08              |
| 3:D:33:ASN:HD21   | 3:D:35:ARG:HG2    | 0.91                     | 1.08              |
| 5:P:368:VAL:HG23  | 5:P:369:LEU:H     | 1.12                     | 1.07              |
| 3:N:675:ARG:HH22  | 5:P:420:ASP:HB3   | 1.11                     | 1.07              |
| 3:N:245:LEU:HA    | 3:N:309:GLY:H     | 1.19                     | 1.07              |
| 2:C:230:ARG:HG2   | 2:C:233:GLU:HG3   | 1.35                     | 1.07              |
| 1:K:12:THR:HA     | 1:L:229:GLN:HB3   | 1.29                     | 1.07              |
| 2:M:762:LYS:HG2   | 2:M:763:GLY:H     | 1.19                     | 1.07              |
| 3:N:407:VAL:HG22  | 3:N:408:GLU:H     | 1.17                     | 1.07              |
| 2:C:776:SER:HA    | 2:C:780:GLU:HB2   | 1.10                     | 1.07              |
| 3:N:36:THR:HB     | 3:N:38:LYS:HG2    | 1.36                     | 1.07              |
| 3:N:361:VAL:HG13  | 3:N:365:ASP:HB3   | 1.28                     | 1.07              |
| 3:D:356:PRO:HB3   | 3:D:440:VAL:HB    | 1.37                     | 1.07              |
| 5:F:280:GLN:HG3   | 5:F:281:GLU:H     | 1.09                     | 1.07              |
| 2:M:250:ARG:HB3   | 2:M:253:ALA:HB2   | 1.36                     | 1.06              |
| 5:F:210:LEU:HA    | 5:F:213:ILE:HD12  | 1.23                     | 1.06              |
| 2:C:368:THR:HB    | 2:C:369:PRO:HD3   | 1.37                     | 1.06              |
| 3:D:182:GLY:HA2   | 3:D:203:ALA:HB3   | 1.31                     | 1.06              |
| 3:N:567:ILE:HG22  | 3:N:571:LYS:HE3   | 1.37                     | 1.06              |
| 3:D:812:ALA:HA    | 3:D:816:HIS:HB2   | 1.37                     | 1.06              |
| 1:A:14:ARG:HD2    | 1:B:234:ALA:H     | 1.14                     | 1.06              |
| 3:N:1286:THR:HG22 | 3:N:1288:GLU:H    | 1.10                     | 1.05              |
| 4:O:41:GLU:HB2    | 4:O:42:PRO:HD2    | 1.35                     | 1.05              |
| 5:P:210:LEU:HA    | 5:P:213:ILE:HD12  | 1.38                     | 1.05              |
| 3:D:1152:GLU:N    | 3:D:1162:GLU:HB3  | 1.72                     | 1.05              |
| 3:N:1217:ILE:H    | 3:N:1217:ILE:HD12 | 1.21                     | 1.05              |
| 3:N:1486:VAL:HG21 | 4:O:22:VAL:HG13   | 1.39                     | 1.05              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:266:GLU:HB3   | 3:N:286:VAL:CG2   | 1.87                     | 1.05              |
| 5:P:278:LEU:HB2   | 5:P:286:PRO:HG3   | 1.36                     | 1.05              |
| 3:D:47:GLU:HB2    | 3:D:51:GLY:O      | 1.57                     | 1.05              |
| 3:N:133:ILE:HG23  | 3:N:456:MET:HE1   | 1.39                     | 1.05              |
| 2:M:772:ARG:HE    | 5:P:373:LYS:HG3   | 1.17                     | 1.05              |
| 3:D:437:VAL:HG11  | 5:F:175:HIS:HB3   | 1.37                     | 1.04              |
| 3:D:227:LEU:HA    | 3:D:331:VAL:HG23  | 1.06                     | 1.04              |
| 2:C:150:PRO:HA    | 2:C:158:TYR:HB3   | 1.07                     | 1.04              |
| 2:C:192:PRO:HB2   | 2:C:195:LEU:HD21  | 1.40                     | 1.04              |
| 3:N:1412:LYS:O    | 3:N:1414:PRO:HD3  | 1.57                     | 1.04              |
| 2:C:195:LEU:HD23  | 2:C:195:LEU:H     | 1.22                     | 1.04              |
| 3:D:1101:VAL:HG21 | 3:D:1424:VAL:HB   | 1.36                     | 1.04              |
| 3:D:253:ALA:H     | 3:D:301:GLY:HA3   | 1.21                     | 1.04              |
| 2:M:650:ARG:H     | 2:M:650:ARG:NE    | 1.55                     | 1.04              |
| 2:C:776:SER:CA    | 2:C:780:GLU:HB2   | 1.86                     | 1.04              |
| 3:D:33:ASN:ND2    | 3:D:35:ARG:HG2    | 1.73                     | 1.04              |
| 2:C:100:LEU:HD23  | 2:C:368:THR:HA    | 1.05                     | 1.03              |
| 1:B:179:PHE:HB3   | 1:B:197:LEU:HD13  | 1.40                     | 1.03              |
| 3:D:804:LEU:HB2   | 3:D:809:PRO:CG    | 1.89                     | 1.03              |
| 2:M:197:LEU:HB3   | 2:M:207:LEU:HD13  | 1.41                     | 1.03              |
| 2:C:15:LEU:HD12   | 2:C:15:LEU:H      | 1.19                     | 1.03              |
| 1:L:101:LEU:HD13  | 1:L:114:PHE:HA    | 1.40                     | 1.03              |
| 2:M:6:PHE:HB3     | 2:M:908:GLY:HA2   | 1.41                     | 1.03              |
| 3:N:1267:ARG:NH1  | 3:N:1267:ARG:HB2  | 1.73                     | 1.03              |
| 2:C:166:PRO:HG2   | 2:C:169:GLY:HA3   | 1.39                     | 1.03              |
| 3:D:951:ILE:HD11  | 3:D:1062:ARG:HG3  | 1.41                     | 1.03              |
| 4:E:6:ILE:HA      | 4:E:9:LEU:HD12    | 1.35                     | 1.03              |
| 1:L:104:GLU:HB3   | 1:L:137:ARG:HG3   | 1.41                     | 1.03              |
| 2:C:1115:LEU:HB3  | 3:D:85:VAL:HG23   | 1.39                     | 1.03              |
| 3:N:121:THR:HG23  | 3:N:122:GLU:H     | 1.19                     | 1.02              |
| 3:N:142:LEU:HB3   | 3:N:146:PRO:HA    | 1.38                     | 1.02              |
| 3:D:957:PRO:HG3   | 3:D:1010:ASN:HD22 | 1.19                     | 1.02              |
| 2:M:274:ARG:HH21  | 2:M:284:ARG:HB3   | 1.22                     | 1.02              |
| 3:N:417:PRO:HB3   | 3:N:430:ASP:HA    | 1.38                     | 1.02              |
| 1:B:188:GLN:HG2   | 1:B:189:ARG:H     | 1.18                     | 1.02              |
| 3:D:820:GLU:HG3   | 3:D:836:VAL:HG11  | 1.40                     | 1.02              |
| 3:N:965:GLU:HG3   | 3:N:969:ARG:HH21  | 1.20                     | 1.02              |
| 5:P:136:LEU:HB3   | 5:P:140:ARG:HD3   | 1.36                     | 1.02              |
| 3:D:660:LYS:HG3   | 3:D:694:VAL:HG22  | 1.37                     | 1.02              |
| 3:D:534:ARG:HH21  | 5:F:313:GLU:HB2   | 1.18                     | 1.02              |
| 2:C:65:VAL:O      | 2:C:100:LEU:HA    | 1.56                     | 1.02              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:988:VAL:HG12  | 3:D:948:THR:HB    | 1.42                     | 1.02              |
| 1:B:101:LEU:HD13  | 1:B:114:PHE:HA    | 1.37                     | 1.02              |
| 3:D:295:GLY:HA2   | 3:D:302:GLN:HB3   | 1.37                     | 1.02              |
| 3:D:433:GLY:HA2   | 3:D:449:SER:H     | 1.20                     | 1.02              |
| 2:M:108:ILE:HB    | 2:M:368:THR:HG21  | 1.40                     | 1.02              |
| 3:N:60:CYS:SG     | 3:N:62:LYS:HG2    | 1.99                     | 1.02              |
| 3:D:1128:VAL:CG2  | 3:D:1131:SER:HB3  | 1.88                     | 1.02              |
| 3:D:1171:VAL:HA   | 3:D:1174:LEU:HD12 | 1.42                     | 1.02              |
| 2:M:1101:THR:HB   | 3:N:5:VAL:HG21    | 1.37                     | 1.02              |
| 2:C:904:PRO:HB2   | 2:C:907:ASP:HB3   | 1.42                     | 1.01              |
| 3:D:554:LEU:HA    | 3:D:557:LEU:HD12  | 1.40                     | 1.01              |
| 3:D:127:LEU:HD23  | 3:D:128:TYR:N     | 1.76                     | 1.01              |
| 2:C:195:LEU:HB2   | 2:C:238:LEU:HD21  | 1.41                     | 1.01              |
| 3:D:411:THR:HB    | 3:D:437:VAL:HB    | 1.39                     | 1.01              |
| 3:N:490:ALA:HA    | 3:N:493:ARG:HE    | 1.25                     | 1.01              |
| 2:C:910:LYS:HG3   | 2:C:912:PRO:HD2   | 1.39                     | 1.01              |
| 3:D:534:ARG:HE    | 5:F:314:PRO:HA    | 1.26                     | 1.01              |
| 2:M:751:PRO:HB3   | 2:M:794:PRO:HA    | 1.42                     | 1.01              |
| 3:N:1033:GLN:CD   | 3:N:1033:GLN:H    | 1.63                     | 1.01              |
| 3:D:284:LEU:HD12  | 3:D:290:PRO:HB3   | 1.43                     | 1.00              |
| 2:C:283:ILE:HG22  | 2:C:284:ARG:H     | 1.20                     | 1.00              |
| 2:C:41:ASN:HA     | 2:C:45:GLN:HB3    | 1.42                     | 1.00              |
| 2:C:542:VAL:HG23  | 2:C:543:ASN:H     | 1.24                     | 1.00              |
| 3:D:355:VAL:HG11  | 3:D:385:VAL:HG21  | 1.41                     | 1.00              |
| 3:N:253:ALA:H     | 3:N:301:GLY:HA3   | 1.26                     | 1.00              |
| 3:N:411:THR:HG21  | 5:P:179:GLU:HG3   | 1.40                     | 1.00              |
| 5:F:214:GLN:HA    | 5:F:217:ASN:HD22  | 1.26                     | 1.00              |
| 2:M:260:LEU:HD13  | 2:M:291:ALA:HB2   | 1.41                     | 1.00              |
| 3:D:440:VAL:HG23  | 3:D:441:ARG:H     | 1.26                     | 1.00              |
| 1:K:188:GLN:HG3   | 1:K:189:ARG:H     | 1.23                     | 1.00              |
| 2:M:580:MET:HB3   | 2:M:584:GLU:CD    | 1.81                     | 1.00              |
| 3:N:147:VAL:HG22  | 3:N:148:GLU:H     | 1.23                     | 1.00              |
| 2:M:175:GLU:HG2   | 2:M:176:VAL:H     | 1.24                     | 1.00              |
| 2:M:230:ARG:NH2   | 2:M:237:ARG:HH22  | 1.58                     | 1.00              |
| 3:N:1098:LEU:HD12 | 3:N:1098:LEU:H    | 1.24                     | 1.00              |
| 2:C:1115:LEU:HD13 | 3:D:85:VAL:HB     | 1.44                     | 0.99              |
| 2:M:194:VAL:HA    | 2:M:197:LEU:HG    | 1.44                     | 0.99              |
| 2:M:413:LEU:HA    | 2:M:419:THR:HG21  | 1.40                     | 0.99              |
| 3:D:148:GLU:HB3   | 3:D:151:GLN:HB2   | 1.44                     | 0.99              |
| 3:N:118:LEU:HA    | 3:N:123:LEU:HD12  | 1.40                     | 0.99              |
| 3:D:206:ARG:HE    | 3:D:394:LEU:HB2   | 1.26                     | 0.99              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:470:PRO:HG3  | 2:M:485:TYR:CZ    | 1.97                     | 0.99              |
| 3:N:843:PHE:HE2  | 3:N:864:VAL:HG11  | 1.26                     | 0.99              |
| 3:D:249:TYR:CE1  | 3:D:330:THR:HG21  | 1.97                     | 0.99              |
| 2:M:230:ARG:HH21 | 2:M:237:ARG:NH2   | 1.58                     | 0.99              |
| 2:C:100:LEU:CD2  | 2:C:368:THR:HA    | 1.93                     | 0.99              |
| 5:F:418:LEU:H    | 5:F:418:LEU:HD12  | 1.27                     | 0.99              |
| 2:M:186:VAL:HG13 | 2:M:187:ASN:H     | 1.28                     | 0.99              |
| 1:L:161:ARG:HB2  | 1:L:164:ALA:HB2   | 1.45                     | 0.99              |
| 2:M:909:ALA:HB1  | 2:M:914:ILE:HD11  | 1.42                     | 0.99              |
| 3:D:361:VAL:HG13 | 3:D:379:ALA:HB1   | 1.44                     | 0.99              |
| 3:D:483:HIS:HB2  | 3:D:484:PRO:HD3   | 1.41                     | 0.99              |
| 2:C:694:LEU:HD21 | 2:C:868:ASP:HB3   | 1.44                     | 0.99              |
| 2:C:737:LEU:HA   | 2:C:743:VAL:HA    | 1.45                     | 0.99              |
| 3:N:254:GLU:O    | 3:N:299:GLU:HB2   | 1.61                     | 0.99              |
| 3:D:1383:ASP:HB3 | 3:D:1416:ALA:H    | 1.24                     | 0.99              |
| 1:L:241:GLU:H    | 1:L:242:PRO:HD2   | 1.27                     | 0.99              |
| 2:M:301:GLU:HA   | 2:M:304:LEU:HD22  | 1.41                     | 0.99              |
| 3:N:826:PRO:O    | 3:N:829:VAL:HG22  | 1.63                     | 0.99              |
| 1:B:104:GLU:HB3  | 1:B:137:ARG:HG3   | 1.41                     | 0.98              |
| 3:D:206:ARG:HH21 | 3:D:394:LEU:HD13  | 1.24                     | 0.98              |
| 3:D:257:GLY:HA2  | 3:D:274:ARG:HA    | 1.43                     | 0.98              |
| 2:M:542:VAL:HG23 | 2:M:543:ASN:H     | 1.26                     | 0.98              |
| 2:M:987:ILE:HG23 | 3:N:948:THR:HG21  | 1.45                     | 0.98              |
| 3:N:274:ARG:HB3  | 3:N:279:VAL:HG21  | 1.45                     | 0.98              |
| 2:C:56:GLU:OE2   | 2:C:356:ARG:HA    | 1.61                     | 0.98              |
| 2:M:243:ARG:HG3  | 2:M:244:PRO:HA    | 1.44                     | 0.98              |
| 3:D:1161:GLU:HG3 | 3:D:1164:ARG:HB2  | 1.43                     | 0.98              |
| 1:A:41:ARG:HA    | 1:A:44:LEU:HD12   | 1.45                     | 0.98              |
| 2:C:257:VAL:HA   | 2:C:261:ILE:HD12  | 1.39                     | 0.98              |
| 5:P:75:ILE:HG13  | 5:P:76:SER:H      | 1.27                     | 0.97              |
| 3:D:227:LEU:HD11 | 3:D:326:GLU:HA    | 1.46                     | 0.97              |
| 3:N:584:ASN:OD1  | 3:N:590:PRO:HD2   | 1.61                     | 0.97              |
| 4:E:40:LEU:HD12  | 4:E:41:GLU:H      | 1.30                     | 0.97              |
| 2:M:226:VAL:HG23 | 2:M:227:PHE:HD1   | 1.30                     | 0.97              |
| 5:F:81:VAL:HG23  | 5:F:82:ARG:H      | 1.28                     | 0.97              |
| 1:L:73:GLU:HG3   | 1:L:130:ALA:HB1   | 1.47                     | 0.97              |
| 2:M:304:LEU:HB3  | 2:M:305:PRO:HD3   | 1.44                     | 0.97              |
| 2:M:690:ILE:HG22 | 2:M:852:ILE:HG23  | 1.46                     | 0.97              |
| 3:N:1171:VAL:HA  | 3:N:1174:LEU:HD12 | 1.45                     | 0.97              |
| 5:P:208:SER:HB3  | 5:P:211:ASP:OD2   | 1.65                     | 0.97              |
| 2:M:1056:LYS:HE2 | 3:N:625:TYR:HB2   | 1.46                     | 0.97              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:343:ASP:HB3   | 5:P:347:GLN:HE22 | 1.30                     | 0.97              |
| 1:B:76:VAL:HA     | 1:B:79:ILE:HD12  | 1.44                     | 0.96              |
| 3:D:1277:ILE:HG22 | 3:D:1278:ASP:H   | 1.29                     | 0.96              |
| 5:F:385:GLU:HA    | 5:F:388:ALA:HB3  | 1.42                     | 0.96              |
| 2:C:238:LEU:O     | 2:C:241:LEU:HG   | 1.64                     | 0.96              |
| 3:D:227:LEU:HA    | 3:D:331:VAL:CG2  | 1.94                     | 0.96              |
| 2:M:257:VAL:HA    | 2:M:261:ILE:HD12 | 1.46                     | 0.96              |
| 2:M:600:ASP:HB3   | 2:M:650:ARG:HA   | 1.45                     | 0.96              |
| 2:C:650:ARG:H     | 2:C:650:ARG:NE   | 1.63                     | 0.96              |
| 3:N:133:ILE:HB    | 3:N:454:ALA:HB1  | 1.46                     | 0.96              |
| 2:C:267:TYR:HB2   | 2:C:272:ALA:CB   | 1.95                     | 0.96              |
| 2:C:363:SER:HB2   | 2:C:366:SER:HB3  | 1.43                     | 0.96              |
| 5:P:214:GLN:HA    | 5:P:217:ASN:HD22 | 1.28                     | 0.96              |
| 1:B:185:ARG:HA    | 1:B:190:THR:HA   | 1.47                     | 0.96              |
| 3:D:137:PRO:HD2   | 3:D:453:ASP:HB3  | 1.48                     | 0.96              |
| 3:D:843:PHE:HE2   | 3:D:864:VAL:HG11 | 1.29                     | 0.96              |
| 2:C:625:LEU:HD11  | 2:C:639:GLN:HB2  | 1.45                     | 0.96              |
| 3:D:245:LEU:H     | 3:D:309:GLY:CA   | 1.77                     | 0.96              |
| 2:C:926:PHE:HE2   | 2:C:960:GLU:HG3  | 1.31                     | 0.96              |
| 2:M:59:LYS:HD2    | 2:M:59:LYS:N     | 1.81                     | 0.95              |
| 3:N:249:TYR:HB3   | 3:N:307:ALA:HB3  | 1.46                     | 0.95              |
| 5:P:368:VAL:HG23  | 5:P:369:LEU:HG   | 1.47                     | 0.95              |
| 1:L:206:THR:HB    | 1:L:209:GLU:HG3  | 1.47                     | 0.95              |
| 2:C:650:ARG:HE    | 2:C:650:ARG:N    | 1.63                     | 0.95              |
| 3:D:139:GLY:O     | 3:D:147:VAL:HB   | 1.65                     | 0.95              |
| 3:N:22:SER:HA     | 3:N:90:MET:O     | 1.66                     | 0.95              |
| 2:M:839:LEU:HD23  | 2:M:996:LYS:HA   | 1.45                     | 0.95              |
| 3:N:1267:ARG:HH21 | 3:N:1271:LYS:HZ1 | 0.99                     | 0.95              |
| 3:N:1341:PRO:HG2  | 3:N:1342:GLU:OE2 | 1.67                     | 0.95              |
| 3:N:540:LEU:HA    | 3:N:543:LEU:HD12 | 1.47                     | 0.95              |
| 2:C:881:ASN:H     | 2:C:881:ASN:HD22 | 0.98                     | 0.95              |
| 3:D:223:LEU:O     | 3:D:332:TYR:HA   | 1.67                     | 0.95              |
| 3:N:542:ASP:O     | 3:N:546:ARG:HG2  | 1.66                     | 0.95              |
| 3:N:827:ILE:HA    | 3:N:836:VAL:HB   | 1.48                     | 0.95              |
| 2:M:93:PRO:HA     | 2:M:117:HIS:HB3  | 1.49                     | 0.95              |
| 3:N:485:SER:O     | 3:N:489:ARG:HD3  | 1.66                     | 0.95              |
| 2:M:21:ILE:HD12   | 2:M:21:ILE:H     | 1.29                     | 0.95              |
| 3:N:217:LYS:HB2   | 3:N:339:TRP:HE1  | 1.30                     | 0.95              |
| 3:D:543:LEU:HA    | 3:D:546:ARG:HD3  | 1.47                     | 0.95              |
| 2:M:368:THR:H     | 2:M:369:PRO:CD   | 1.80                     | 0.94              |
| 3:D:30:GLU:HB3    | 3:D:40:GLU:HG2   | 1.48                     | 0.94              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:417:PRO:HB2  | 3:D:428:LYS:HG2  | 1.49                     | 0.94              |
| 3:D:249:TYR:CB   | 3:D:307:ALA:HB3  | 1.97                     | 0.94              |
| 3:D:248:PRO:HA   | 3:D:308:LYS:HZ3  | 1.31                     | 0.94              |
| 5:F:215:GLU:O    | 5:F:218:GLN:HG3  | 1.67                     | 0.94              |
| 2:M:474:VAL:HG12 | 2:M:530:GLU:O    | 1.66                     | 0.94              |
| 3:D:408:GLU:OE2  | 3:D:421:LEU:HG   | 1.68                     | 0.94              |
| 1:A:39:PRO:HG3   | 1:B:39:PRO:HG3   | 1.49                     | 0.94              |
| 3:N:654:LYS:HB3  | 3:N:655:PRO:HD3  | 1.46                     | 0.94              |
| 2:C:31:GLN:HG2   | 2:C:35:PRO:CB    | 1.97                     | 0.94              |
| 3:D:187:LYS:HG3  | 3:D:198:ARG:HG3  | 1.50                     | 0.94              |
| 3:D:485:SER:O    | 3:D:489:ARG:HD3  | 1.67                     | 0.94              |
| 2:C:38:LYS:HG3   | 2:C:39:ARG:H     | 1.32                     | 0.94              |
| 3:D:147:VAL:HG22 | 3:D:148:GLU:H    | 1.32                     | 0.94              |
| 3:N:349:PRO:HB2  | 5:P:232:ARG:HH22 | 1.32                     | 0.94              |
| 1:A:76:VAL:HA    | 1:A:79:ILE:HD12  | 1.49                     | 0.94              |
| 5:F:392:VAL:HG11 | 5:F:396:ARG:HD3  | 1.49                     | 0.94              |
| 1:L:235:ALA:HB3  | 1:L:236:PRO:HD3  | 1.50                     | 0.94              |
| 3:D:1353:GLN:O   | 3:D:1357:ARG:HG2 | 1.68                     | 0.94              |
| 3:D:421:LEU:HD23 | 3:D:427:VAL:HG12 | 1.47                     | 0.94              |
| 3:D:631:ILE:HG21 | 3:D:745:MET:HG3  | 1.48                     | 0.94              |
| 3:D:928:ALA:HA   | 3:D:931:LEU:HD12 | 1.50                     | 0.93              |
| 1:K:110:LYS:HB2  | 1:K:112:ARG:HG2  | 1.48                     | 0.93              |
| 3:N:127:LEU:HD23 | 3:N:128:TYR:N    | 1.83                     | 0.93              |
| 3:D:188:GLY:N    | 3:D:198:ARG:HA   | 1.82                     | 0.93              |
| 2:M:230:ARG:NE   | 2:M:233:GLU:HG2  | 1.83                     | 0.93              |
| 3:N:15:PRO:HA    | 3:N:18:ILE:HD12  | 1.50                     | 0.93              |
| 2:M:1058:ASP:OD2 | 2:M:1084:SER:HB3 | 1.69                     | 0.93              |
| 2:M:31:GLN:HG2   | 2:M:35:PRO:HB3   | 1.48                     | 0.93              |
| 2:C:503:LEU:HD12 | 2:C:508:ILE:HA   | 1.50                     | 0.93              |
| 2:M:1047:HIS:O   | 2:M:1051:GLU:HG2 | 1.68                     | 0.93              |
| 3:N:906:GLN:HB3  | 3:N:911:LEU:HD21 | 1.47                     | 0.93              |
| 2:C:21:ILE:HD12  | 2:C:21:ILE:H     | 1.30                     | 0.93              |
| 3:D:543:LEU:O    | 3:D:546:ARG:HG3  | 1.67                     | 0.93              |
| 5:F:379:ARG:HD3  | 5:F:380:GLU:HB2  | 1.50                     | 0.93              |
| 5:F:282:LEU:HG   | 5:F:284:ARG:HG2  | 1.49                     | 0.93              |
| 3:N:931:LEU:HA   | 3:N:934:LEU:HD12 | 1.49                     | 0.93              |
| 2:C:654:LEU:HD12 | 2:C:655:LEU:H    | 1.33                     | 0.92              |
| 2:C:751:PRO:HB3  | 2:C:794:PRO:HA   | 1.51                     | 0.92              |
| 3:N:535:PHE:O    | 5:P:314:PRO:HB2  | 1.69                     | 0.92              |
| 2:C:182:VAL:HB   | 2:C:193:LEU:H    | 1.34                     | 0.92              |
| 2:M:397:GLU:H    | 2:M:633:GLN:HE21 | 1.18                     | 0.92              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:112:ARG:NH1   | 1:B:112:ARG:HB3   | 1.84                     | 0.92              |
| 2:C:115:LEU:HD11  | 2:C:373:VAL:HG12  | 1.49                     | 0.92              |
| 2:C:909:ALA:HB1   | 2:C:914:ILE:HD11  | 1.48                     | 0.92              |
| 3:D:954:ALA:HB3   | 3:D:1062:ARG:HD2  | 1.52                     | 0.92              |
| 3:D:128:TYR:HD1   | 3:D:457:GLY:HA2   | 1.35                     | 0.92              |
| 1:K:122:ILE:HG22  | 1:K:124:ASN:H     | 1.30                     | 0.92              |
| 3:D:1172:HIS:HA   | 3:D:1175:ILE:HD12 | 1.48                     | 0.92              |
| 3:N:1498:ALA:HB3  | 4:O:84:ARG:CZ     | 2.00                     | 0.92              |
| 3:N:348:GLN:H     | 3:N:351:MET:HE2   | 1.30                     | 0.92              |
| 3:N:699:VAL:HG12  | 3:N:717:GLN:HG2   | 1.49                     | 0.92              |
| 1:B:41:ARG:HA     | 1:B:44:LEU:HD12   | 1.49                     | 0.92              |
| 3:D:1128:VAL:HG21 | 3:D:1131:SER:HB3  | 1.48                     | 0.92              |
| 3:D:957:PRO:HG2   | 3:D:1007:VAL:HA   | 1.52                     | 0.92              |
| 2:M:1101:THR:HB   | 3:N:5:VAL:CG2     | 1.99                     | 0.92              |
| 2:C:166:PRO:HG2   | 2:C:169:GLY:CA    | 2.00                     | 0.92              |
| 3:N:358:GLY:HA2   | 3:N:385:VAL:HB    | 1.51                     | 0.92              |
| 3:N:553:ARG:HH12  | 5:P:211:ASP:HA    | 1.33                     | 0.92              |
| 2:M:503:LEU:HD12  | 2:M:508:ILE:HA    | 1.50                     | 0.92              |
| 3:N:297:ILE:HG23  | 3:N:298:VAL:H     | 1.35                     | 0.92              |
| 3:N:806:PHE:HA    | 3:N:809:PRO:HD2   | 1.49                     | 0.92              |
| 3:D:118:LEU:HA    | 3:D:123:LEU:HD12  | 1.52                     | 0.92              |
| 3:D:1405:GLU:O    | 3:D:1412:LYS:HA   | 1.70                     | 0.92              |
| 1:K:152:PRO:HG2   | 1:K:155:LYS:HB2   | 1.50                     | 0.92              |
| 3:N:131:LYS:HA    | 3:N:456:MET:HG3   | 1.52                     | 0.92              |
| 3:N:82:LYS:HB2    | 3:N:84:ILE:HG22   | 1.50                     | 0.92              |
| 1:B:38:ASN:HB3    | 1:B:39:PRO:HD3    | 1.51                     | 0.91              |
| 1:L:137:ARG:HH12  | 1:L:139:ASN:HB2   | 1.33                     | 0.91              |
| 2:M:1058:ASP:O    | 2:M:1083:GLU:HG2  | 1.70                     | 0.91              |
| 2:M:325:ILE:HD12  | 2:M:325:ILE:H     | 1.34                     | 0.91              |
| 3:D:253:ALA:H     | 3:D:301:GLY:CA    | 1.84                     | 0.91              |
| 3:D:930:LEU:HG    | 3:D:934:LEU:HD11  | 1.53                     | 0.91              |
| 3:N:368:VAL:HB    | 3:N:377:VAL:HG21  | 1.50                     | 0.91              |
| 3:N:138:LYS:HB3   | 3:N:450:TYR:OH    | 1.67                     | 0.91              |
| 3:N:565:ILE:HG23  | 3:N:566:ILE:H     | 1.33                     | 0.91              |
| 2:C:1104:GLU:HA   | 3:D:7:LYS:NZ      | 1.86                     | 0.91              |
| 1:L:197:LEU:HD12  | 1:L:198:ARG:H     | 1.33                     | 0.91              |
| 3:N:408:GLU:HB3   | 3:N:422:ALA:HB2   | 1.50                     | 0.91              |
| 2:C:305:PRO:HA    | 2:C:308:ARG:NE    | 1.86                     | 0.91              |
| 3:D:313:MET:SD    | 3:D:314:PRO:HD2   | 2.10                     | 0.91              |
| 2:M:185:LYS:HG2   | 2:M:190:LYS:HD3   | 1.50                     | 0.91              |
| 1:L:233:VAL:O     | 1:L:236:PRO:HD2   | 1.69                     | 0.91              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:238:LEU:O    | 2:M:241:LEU:HG    | 1.71                     | 0.91              |
| 2:M:264:PRO:HB2  | 2:M:289:THR:CG2   | 2.01                     | 0.91              |
| 3:N:800:LYS:HD2  | 3:N:800:LYS:C     | 1.91                     | 0.91              |
| 1:A:34:VAL:HB    | 1:B:42:ARG:NH1    | 1.85                     | 0.91              |
| 2:C:317:VAL:N    | 2:C:318:PRO:HD3   | 1.85                     | 0.91              |
| 3:N:1345:GLU:HA  | 3:N:1348:LEU:HD12 | 1.51                     | 0.91              |
| 2:C:72:ARG:CG    | 2:C:95:TYR:HB2    | 2.01                     | 0.91              |
| 3:D:133:ILE:HG23 | 3:D:456:MET:HG3   | 1.50                     | 0.91              |
| 3:D:610:LYS:NZ   | 3:D:1442:ASN:H    | 1.68                     | 0.91              |
| 3:D:245:LEU:H    | 3:D:309:GLY:HA2   | 1.34                     | 0.91              |
| 4:E:37:ASN:N     | 4:E:37:ASN:HD22   | 1.69                     | 0.91              |
| 5:F:189:GLU:HA   | 5:F:192:LEU:HG    | 1.50                     | 0.91              |
| 2:M:628:PHE:HD1  | 2:M:628:PHE:H     | 1.17                     | 0.91              |
| 5:P:343:ASP:HB3  | 5:P:347:GLN:NE2   | 1.86                     | 0.91              |
| 3:D:417:PRO:HB3  | 3:D:430:ASP:N     | 1.85                     | 0.91              |
| 3:N:484:PRO:O    | 3:N:489:ARG:HB2   | 1.71                     | 0.91              |
| 2:C:910:LYS:HG2  | 2:C:913:GLU:HG3   | 1.50                     | 0.90              |
| 3:D:137:PRO:CD   | 3:D:453:ASP:HB3   | 2.01                     | 0.90              |
| 1:K:76:VAL:HA    | 1:K:79:ILE:HD12   | 1.52                     | 0.90              |
| 3:D:416:ALA:HB2  | 3:D:432:TYR:CA    | 2.00                     | 0.90              |
| 2:M:1038:TRP:HA  | 2:M:1041:GLU:OE1  | 1.70                     | 0.90              |
| 2:C:150:PRO:HA   | 2:C:158:TYR:CB    | 1.98                     | 0.90              |
| 2:C:186:VAL:HG23 | 2:C:187:ASN:H     | 1.33                     | 0.90              |
| 2:C:759:THR:HB   | 2:C:785:VAL:HG12  | 1.53                     | 0.90              |
| 1:K:206:THR:HB   | 1:K:209:GLU:HG3   | 1.52                     | 0.90              |
| 2:M:585:GLU:O    | 2:M:588:VAL:HG22  | 1.71                     | 0.90              |
| 2:C:776:SER:HA   | 2:C:780:GLU:CB    | 2.00                     | 0.90              |
| 1:L:73:GLU:HG3   | 1:L:130:ALA:CB    | 2.01                     | 0.90              |
| 2:C:415:PRO:HB2  | 2:C:418:LEU:HB2   | 1.51                     | 0.90              |
| 3:D:1489:GLN:HA  | 3:D:1492:LEU:CG   | 2.01                     | 0.90              |
| 2:M:679:PHE:HA   | 3:N:943:THR:HG23  | 1.52                     | 0.90              |
| 1:B:212:ASN:O    | 1:B:215:VAL:HG22  | 1.72                     | 0.90              |
| 1:B:235:ALA:HB3  | 1:B:236:PRO:HD3   | 1.53                     | 0.90              |
| 3:D:243:ALA:HB3  | 3:D:311:LEU:HD12  | 1.52                     | 0.90              |
| 3:D:820:GLU:HG3  | 3:D:836:VAL:CG1   | 2.00                     | 0.90              |
| 2:C:115:LEU:HD11 | 2:C:373:VAL:HG11  | 1.53                     | 0.90              |
| 1:L:58:ILE:HG12  | 1:L:140:MET:CB    | 2.02                     | 0.90              |
| 1:L:36:LEU:O     | 1:L:39:PRO:HD2    | 1.72                     | 0.90              |
| 2:M:15:LEU:N     | 2:M:15:LEU:HD12   | 1.87                     | 0.90              |
| 3:N:147:VAL:HG22 | 3:N:148:GLU:N     | 1.86                     | 0.90              |
| 3:N:217:LYS:HB2  | 3:N:339:TRP:NE1   | 1.86                     | 0.90              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:241:ILE:HD13 | 3:N:310:LEU:HD22 | 1.52                     | 0.90              |
| 5:P:367:MET:HB2  | 5:P:371:LEU:HG   | 1.53                     | 0.90              |
| 1:A:226:SER:O    | 1:A:228:PRO:HD3  | 1.72                     | 0.90              |
| 3:D:367:ILE:HB   | 3:D:377:VAL:HG12 | 1.53                     | 0.90              |
| 2:M:15:LEU:H     | 2:M:15:LEU:CD1   | 1.78                     | 0.90              |
| 3:N:219:GLU:HG2  | 3:N:220:ARG:H    | 1.35                     | 0.90              |
| 3:N:52:PRO:O     | 3:N:86:ARG:HD2   | 1.71                     | 0.90              |
| 5:F:265:VAL:HA   | 5:F:268:ILE:HD12 | 1.54                     | 0.90              |
| 3:N:249:TYR:CB   | 3:N:307:ALA:HB3  | 2.01                     | 0.90              |
| 3:N:322:VAL:HA   | 3:N:335:LEU:CG   | 2.01                     | 0.90              |
| 2:C:290:LEU:HD22 | 2:C:302:VAL:HG21 | 1.51                     | 0.90              |
| 3:D:368:VAL:HB   | 3:D:377:VAL:CG2  | 2.01                     | 0.90              |
| 2:M:958:THR:HG23 | 2:M:961:GLU:HB2  | 1.53                     | 0.90              |
| 2:C:1000:MET:HB3 | 2:C:1002:GLU:HG3 | 1.53                     | 0.89              |
| 3:D:1481:VAL:CG1 | 4:E:18:ARG:HA    | 2.02                     | 0.89              |
| 1:L:143:ARG:HD3  | 1:L:144:VAL:N    | 1.85                     | 0.89              |
| 1:B:151:VAL:HB   | 1:B:169:ALA:HB3  | 1.53                     | 0.89              |
| 2:C:676:ILE:HG23 | 2:C:988:VAL:HG13 | 1.55                     | 0.89              |
| 4:E:41:GLU:HB2   | 4:E:42:PRO:HD2   | 1.53                     | 0.89              |
| 3:N:410:SER:HB3  | 5:P:175:HIS:ND1  | 1.88                     | 0.89              |
| 2:C:59:LYS:N     | 2:C:59:LYS:HD2   | 1.88                     | 0.89              |
| 5:P:321:ILE:HG13 | 5:P:332:PHE:CE1  | 2.08                     | 0.89              |
| 1:A:86:VAL:HG12  | 1:A:124:ASN:HD21 | 1.35                     | 0.89              |
| 2:C:516:ARG:HA   | 2:C:520:GLU:O    | 1.72                     | 0.89              |
| 3:D:266:GLU:HB2  | 3:D:314:PRO:HG3  | 1.55                     | 0.89              |
| 2:M:230:ARG:O    | 2:M:233:GLU:HG3  | 1.70                     | 0.89              |
| 5:P:413:SER:HA   | 5:P:416:ARG:CZ   | 2.03                     | 0.89              |
| 2:C:151:ASP:H    | 2:C:158:TYR:HA   | 1.38                     | 0.89              |
| 3:D:387:LEU:H    | 3:D:387:LEU:HD12 | 1.36                     | 0.89              |
| 1:K:9:PRO:HG3    | 1:K:27:PRO:O     | 1.70                     | 0.89              |
| 5:P:265:VAL:HA   | 5:P:268:ILE:HD12 | 1.54                     | 0.89              |
| 3:D:227:LEU:CA   | 3:D:331:VAL:HG23 | 2.01                     | 0.89              |
| 3:D:811:GLU:O    | 3:D:815:ALA:HB3  | 1.72                     | 0.89              |
| 3:N:322:VAL:CA   | 3:N:335:LEU:HG   | 2.03                     | 0.89              |
| 1:B:161:ARG:HB2  | 1:B:164:ALA:HB2  | 1.55                     | 0.89              |
| 2:C:150:PRO:CA   | 2:C:158:TYR:HB3  | 1.98                     | 0.89              |
| 3:D:136:ASP:HB3  | 3:D:137:PRO:HD3  | 1.54                     | 0.89              |
| 3:D:230:TRP:HE1  | 3:D:233:LYS:HG3  | 1.37                     | 0.89              |
| 2:M:41:ASN:HA    | 2:M:45:GLN:HB3   | 1.55                     | 0.89              |
| 2:C:504:GLU:O    | 2:C:507:ARG:HD2  | 1.72                     | 0.89              |
| 2:M:267:TYR:HB2  | 2:M:272:ALA:HB3  | 1.54                     | 0.89              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:79:GLU:HG2    | 3:D:80:VAL:N      | 1.88                     | 0.89              |
| 1:L:214:ALA:HA    | 1:L:217:ILE:HD12  | 1.53                     | 0.89              |
| 2:C:325:ILE:HD12  | 2:C:325:ILE:H     | 1.38                     | 0.89              |
| 2:M:698:ASP:HA    | 2:M:832:LYS:HE3   | 1.53                     | 0.89              |
| 3:N:1277:ILE:HG22 | 3:N:1278:ASP:H    | 1.35                     | 0.89              |
| 3:N:285:PRO:HB2   | 3:N:312:ARG:O     | 1.72                     | 0.89              |
| 3:D:1407:LEU:O    | 3:D:1410:GLU:HG2  | 1.73                     | 0.88              |
| 5:F:101:GLU:HA    | 5:F:104:ARG:NH1   | 1.87                     | 0.88              |
| 2:M:283:ILE:CG2   | 2:M:284:ARG:H     | 1.86                     | 0.88              |
| 3:N:826:PRO:HD2   | 3:N:829:VAL:HG11  | 1.55                     | 0.88              |
| 2:M:958:THR:HG23  | 2:M:961:GLU:CB    | 2.02                     | 0.88              |
| 5:F:368:VAL:HG23  | 5:F:369:LEU:H     | 1.39                     | 0.88              |
| 2:M:283:ILE:HG22  | 2:M:284:ARG:N     | 1.86                     | 0.88              |
| 3:N:1267:ARG:HE   | 3:N:1271:LYS:HZ2  | 1.19                     | 0.88              |
| 3:N:483:HIS:HB2   | 3:N:484:PRO:CD    | 2.03                     | 0.88              |
| 3:D:1095:THR:O    | 3:D:1099:VAL:HG23 | 1.73                     | 0.88              |
| 3:D:79:GLU:HG2    | 3:D:80:VAL:H      | 1.37                     | 0.88              |
| 2:C:626:ARG:HG3   | 2:C:629:TYR:HD1   | 1.37                     | 0.88              |
| 3:D:530:VAL:HG23  | 3:D:531:ASP:N     | 1.88                     | 0.88              |
| 3:D:584:ASN:OD1   | 3:D:590:PRO:HD2   | 1.73                     | 0.88              |
| 2:C:23:VAL:HA     | 2:C:121:MET:CE    | 2.04                     | 0.88              |
| 2:C:269:LEU:HD12  | 2:C:288:ARG:HB3   | 1.55                     | 0.88              |
| 2:C:304:LEU:HB3   | 2:C:305:PRO:CD    | 2.03                     | 0.88              |
| 3:D:237:LYS:HB3   | 3:D:238:PRO:CD    | 2.03                     | 0.88              |
| 2:M:44:ILE:HG23   | 2:M:344:PHE:HE1   | 1.37                     | 0.88              |
| 2:M:413:LEU:HA    | 2:M:419:THR:CG2   | 2.02                     | 0.88              |
| 2:M:781:LYS:HA    | 2:M:781:LYS:HE2   | 1.53                     | 0.88              |
| 3:N:845:ASN:HB2   | 3:N:848:GLU:HB2   | 1.56                     | 0.88              |
| 2:C:762:LYS:HG2   | 2:C:763:GLY:H     | 1.39                     | 0.88              |
| 3:D:238:PRO:HB3   | 3:D:317:VAL:O     | 1.73                     | 0.88              |
| 2:M:603:VAL:HG23  | 2:M:647:GLN:O     | 1.74                     | 0.88              |
| 3:N:130:SER:HB3   | 3:N:132:TYR:CE1   | 2.08                     | 0.88              |
| 3:N:1495:ILE:O    | 3:N:1499:ARG:HB2  | 1.72                     | 0.88              |
| 2:C:157:ARG:HG3   | 2:C:158:TYR:H     | 1.39                     | 0.88              |
| 3:D:260:GLU:HB2   | 3:D:271:VAL:HB    | 1.55                     | 0.88              |
| 1:L:58:ILE:HG23   | 1:L:139:ASN:O     | 1.74                     | 0.88              |
| 3:N:416:ALA:HB2   | 3:N:432:TYR:CA    | 2.02                     | 0.88              |
| 3:D:806:PHE:HA    | 3:D:809:PRO:HD2   | 1.53                     | 0.88              |
| 3:D:249:TYR:HB3   | 3:D:307:ALA:CB    | 2.00                     | 0.88              |
| 2:M:277:ALA:HB1   | 2:M:281:LEU:HD12  | 1.56                     | 0.88              |
| 2:M:38:LYS:HG3    | 2:M:39:ARG:H      | 1.37                     | 0.88              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:592:THR:HG23  | 3:N:600:LEU:HD21 | 1.56                     | 0.88              |
| 3:N:805:GLU:HA    | 3:N:831:GLY:HA2  | 1.55                     | 0.88              |
| 2:C:185:LYS:HG2   | 2:C:190:LYS:HD3  | 1.54                     | 0.87              |
| 2:M:1056:LYS:HD3  | 3:N:623:VAL:HG13 | 1.55                     | 0.87              |
| 3:N:79:GLU:HG2    | 3:N:80:VAL:H     | 1.38                     | 0.87              |
| 1:B:32:PHE:HA     | 1:B:35:THR:HB    | 1.56                     | 0.87              |
| 2:C:401:LEU:HD11  | 2:C:543:ASN:HB3  | 1.55                     | 0.87              |
| 3:D:552:ASN:HA    | 3:D:555:LYS:HD2  | 1.54                     | 0.87              |
| 5:F:261:PRO:O     | 5:F:264:MET:HB2  | 1.74                     | 0.87              |
| 2:M:317:VAL:N     | 2:M:318:PRO:HD3  | 1.89                     | 0.87              |
| 3:N:136:ASP:HB2   | 3:N:137:PRO:HD3  | 1.53                     | 0.87              |
| 5:F:280:GLN:HG3   | 5:F:281:GLU:N    | 1.87                     | 0.87              |
| 3:N:1394:VAL:HB   | 3:N:1397:LYS:HD2 | 1.54                     | 0.87              |
| 3:N:349:PRO:HB2   | 5:P:232:ARG:NH2  | 1.88                     | 0.87              |
| 3:N:864:VAL:HG12  | 3:N:865:THR:H    | 1.38                     | 0.87              |
| 3:N:912:LYS:HB3   | 3:N:912:LYS:HZ3  | 1.38                     | 0.87              |
| 3:D:223:LEU:HG    | 3:D:224:ARG:H    | 1.37                     | 0.87              |
| 1:K:152:PRO:HB2   | 1:K:154:GLU:OE1  | 1.73                     | 0.87              |
| 2:M:352:ALA:HA    | 2:M:355:VAL:HG12 | 1.56                     | 0.87              |
| 3:N:227:LEU:HA    | 3:N:331:VAL:CG2  | 2.03                     | 0.87              |
| 5:F:80:PRO:HA     | 5:F:83:GLN:HE21  | 1.39                     | 0.87              |
| 5:F:263:HIS:HA    | 5:F:266:GLU:OE2  | 1.73                     | 0.87              |
| 2:C:186:VAL:HG23  | 2:C:187:ASN:N    | 1.86                     | 0.87              |
| 3:D:1031:ASN:H    | 3:D:1034:GLN:NE2 | 1.72                     | 0.87              |
| 2:M:776:SER:HB3   | 5:P:379:ARG:HH22 | 1.38                     | 0.87              |
| 2:C:603:VAL:HG23  | 2:C:647:GLN:O    | 1.75                     | 0.87              |
| 4:E:37:ASN:H      | 4:E:37:ASN:ND2   | 1.70                     | 0.87              |
| 1:L:106:PRO:HA    | 1:L:133:GLU:HA   | 1.54                     | 0.87              |
| 3:N:119:SER:H     | 3:N:123:LEU:CG   | 1.87                     | 0.87              |
| 3:N:1213:ARG:HH11 | 3:N:1213:ARG:HG2 | 1.40                     | 0.87              |
| 5:P:373:LYS:HD2   | 5:P:374:GLY:N    | 1.90                     | 0.87              |
| 3:D:1307:LYS:H    | 3:D:1307:LYS:HE3 | 1.38                     | 0.87              |
| 3:D:1372:VAL:HA   | 3:D:1375:MET:CE  | 2.05                     | 0.87              |
| 3:D:1494:ALA:HB1  | 4:E:88:GLU:HB3   | 1.57                     | 0.87              |
| 3:D:548:ILE:HG22  | 3:D:552:ASN:HD21 | 1.38                     | 0.87              |
| 2:M:250:ARG:CB    | 2:M:253:ALA:HB2  | 2.05                     | 0.87              |
| 3:N:288:MET:HE1   | 3:N:307:ALA:HB2  | 1.56                     | 0.87              |
| 3:N:553:ARG:HH11  | 5:P:214:GLN:HB2  | 1.40                     | 0.87              |
| 1:B:188:GLN:HG2   | 1:B:189:ARG:N    | 1.90                     | 0.86              |
| 1:B:58:ILE:HG12   | 1:B:139:ASN:O    | 1.75                     | 0.86              |
| 3:D:433:GLY:HA2   | 3:D:449:SER:N    | 1.90                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:108:GLU:HG3   | 1:L:131:THR:HG22  | 1.57                     | 0.86              |
| 2:M:694:LEU:HD21  | 2:M:868:ASP:HB3   | 1.54                     | 0.86              |
| 3:N:1353:GLN:O    | 3:N:1357:ARG:HG2  | 1.74                     | 0.86              |
| 3:D:127:LEU:HD22  | 3:D:461:ILE:HD11  | 1.57                     | 0.86              |
| 3:N:237:LYS:HB3   | 3:N:238:PRO:CD    | 2.04                     | 0.86              |
| 3:D:259:VAL:HA    | 3:D:270:LEU:HD11  | 1.54                     | 0.86              |
| 2:M:302:VAL:O     | 2:M:305:PRO:HD2   | 1.74                     | 0.86              |
| 3:N:1312:LEU:HB3  | 3:N:1325:LEU:O    | 1.75                     | 0.86              |
| 3:N:843:PHE:CE2   | 3:N:864:VAL:HG11  | 2.10                     | 0.86              |
| 3:D:188:GLY:H     | 3:D:198:ARG:CA    | 1.86                     | 0.86              |
| 2:M:368:THR:H     | 2:M:369:PRO:HD3   | 1.40                     | 0.86              |
| 3:N:257:GLY:HA2   | 3:N:274:ARG:HA    | 1.56                     | 0.86              |
| 2:C:243:ARG:HG3   | 2:C:244:PRO:HA    | 1.55                     | 0.86              |
| 3:D:417:PRO:HB3   | 3:D:430:ASP:HA    | 1.58                     | 0.86              |
| 3:N:356:PRO:HB3   | 3:N:440:VAL:HB    | 1.58                     | 0.86              |
| 5:P:352:GLU:HA    | 5:P:355:GLU:OE2   | 1.74                     | 0.86              |
| 5:F:289:GLU:CD    | 5:F:289:GLU:H     | 1.79                     | 0.86              |
| 2:M:1085:PHE:O    | 2:M:1088:LEU:HB3  | 1.75                     | 0.86              |
| 3:N:808:THR:H     | 3:N:809:PRO:CD    | 1.88                     | 0.86              |
| 2:M:1005:MET:HG2  | 3:N:629:SER:HB2   | 1.57                     | 0.86              |
| 3:N:10:ILE:O      | 3:N:1454:GLY:HA2  | 1.75                     | 0.86              |
| 3:N:411:THR:HG21  | 5:P:179:GLU:CG    | 2.04                     | 0.86              |
| 5:P:282:LEU:HG    | 5:P:284:ARG:CG    | 2.03                     | 0.86              |
| 2:C:93:PRO:HG3    | 2:C:117:HIS:HD2   | 1.40                     | 0.86              |
| 2:C:157:ARG:HD2   | 2:C:314:THR:HG22  | 1.55                     | 0.86              |
| 3:D:210:ARG:HB2   | 3:D:389:GLU:HG3   | 1.54                     | 0.86              |
| 3:D:438:ASP:OD1   | 3:D:440:VAL:HG22  | 1.75                     | 0.86              |
| 3:N:1099:VAL:HG12 | 10:N:1528:NE6:H14 | 1.58                     | 0.86              |
| 3:N:243:ALA:HB3   | 3:N:311:LEU:HD12  | 1.57                     | 0.86              |
| 2:M:226:VAL:HG23  | 2:M:227:PHE:CD1   | 2.10                     | 0.86              |
| 3:N:1406:ARG:HD3  | 3:N:1412:LYS:NZ   | 1.90                     | 0.86              |
| 2:C:23:VAL:HA     | 2:C:121:MET:HE1   | 1.58                     | 0.86              |
| 2:C:605:LYS:HB3   | 2:C:610:ARG:NH2   | 1.88                     | 0.86              |
| 3:N:1267:ARG:HH11 | 3:N:1267:ARG:HB2  | 1.41                     | 0.86              |
| 2:M:1051:GLU:HG3  | 2:M:1052:MET:H    | 1.40                     | 0.85              |
| 3:N:1341:PRO:O    | 3:N:1344:VAL:HG12 | 1.74                     | 0.85              |
| 3:D:1029:ARG:HH11 | 3:D:1029:ARG:HG3  | 1.40                     | 0.85              |
| 3:N:441:ARG:HG3   | 3:N:443:VAL:HG23  | 1.59                     | 0.85              |
| 1:A:138:LEU:HD12  | 1:A:139:ASN:H     | 1.41                     | 0.85              |
| 3:D:295:GLY:CA    | 3:D:302:GLN:HB3   | 2.06                     | 0.85              |
| 3:D:348:GLN:H     | 3:D:351:MET:HE2   | 1.40                     | 0.85              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:521:PRO:HD2   | 3:D:524:LEU:HD12  | 1.57                     | 0.85              |
| 1:A:38:ASN:HB3    | 1:A:39:PRO:HD3    | 1.57                     | 0.85              |
| 2:M:1088:LEU:HA   | 2:M:1091:GLU:OE1  | 1.76                     | 0.85              |
| 2:C:352:ALA:HA    | 2:C:355:VAL:HG12  | 1.58                     | 0.85              |
| 2:M:878:SER:HA    | 3:N:1034:GLN:OE1  | 1.76                     | 0.85              |
| 3:N:1404:ASN:HA   | 3:N:1408:ILE:HB   | 1.56                     | 0.85              |
| 5:P:138:SER:O     | 5:P:141:VAL:HG22  | 1.76                     | 0.85              |
| 5:P:367:MET:HB3   | 5:P:370:LYS:HE2   | 1.58                     | 0.85              |
| 2:C:1064:ASN:HA   | 5:F:341:PRO:HB3   | 1.56                     | 0.85              |
| 2:C:881:ASN:H     | 2:C:881:ASN:ND2   | 1.75                     | 0.85              |
| 3:D:1489:GLN:CA   | 3:D:1492:LEU:HG   | 2.06                     | 0.85              |
| 3:D:95:LEU:HB2    | 3:D:515:GLU:HA    | 1.58                     | 0.85              |
| 3:D:658:LEU:CA    | 3:D:661:MET:HE3   | 2.06                     | 0.85              |
| 3:N:1018:ASN:O    | 3:N:1022:VAL:HG23 | 1.76                     | 0.85              |
| 1:B:106:PRO:HA    | 1:B:133:GLU:HA    | 1.58                     | 0.85              |
| 3:D:367:ILE:HB    | 3:D:377:VAL:CG1   | 2.06                     | 0.85              |
| 2:M:230:ARG:HG2   | 2:M:233:GLU:CG    | 2.07                     | 0.85              |
| 2:M:649:VAL:HA    | 2:M:650:ARG:HH21  | 1.41                     | 0.85              |
| 3:N:1400:VAL:HG12 | 3:N:1404:ASN:HD21 | 1.42                     | 0.85              |
| 1:B:36:LEU:O      | 1:B:39:PRO:HD2    | 1.77                     | 0.85              |
| 2:C:737:LEU:HD12  | 2:C:743:VAL:N     | 1.91                     | 0.85              |
| 3:N:106:LYS:HE2   | 3:N:106:LYS:HA    | 1.58                     | 0.85              |
| 2:C:1071:ILE:O    | 3:D:659:LYS:HD3   | 1.76                     | 0.85              |
| 3:D:352:ASN:C     | 3:D:368:VAL:HG13  | 1.97                     | 0.85              |
| 3:D:860:LEU:HA    | 3:D:877:PRO:HB2   | 1.58                     | 0.85              |
| 2:M:146:VAL:HG22  | 2:M:162:ILE:HG12  | 1.58                     | 0.85              |
| 2:C:640:ARG:HD2   | 2:C:642:ARG:HH22  | 1.41                     | 0.84              |
| 1:K:90:LEU:HD12   | 1:K:119:ASP:HA    | 1.58                     | 0.84              |
| 2:M:264:PRO:CB    | 2:M:289:THR:HG21  | 2.06                     | 0.84              |
| 2:M:448:ASN:HA    | 2:M:451:LEU:HD12  | 1.59                     | 0.84              |
| 3:N:826:PRO:HB2   | 3:N:829:VAL:HG13  | 1.57                     | 0.84              |
| 5:P:132:ARG:NH2   | 5:P:184:ARG:HH12  | 1.74                     | 0.84              |
| 3:D:261:LEU:HA    | 3:D:269:PHE:O     | 1.76                     | 0.84              |
| 3:D:417:PRO:HB3   | 3:D:430:ASP:CA    | 2.07                     | 0.84              |
| 5:F:355:GLU:HA    | 5:F:358:LEU:HB3   | 1.56                     | 0.84              |
| 3:N:565:ILE:HD13  | 5:P:192:LEU:HD13  | 1.58                     | 0.84              |
| 3:N:168:THR:HG21  | 5:P:93:LEU:HD22   | 1.59                     | 0.84              |
| 3:N:806:PHE:CG    | 3:N:809:PRO:HB2   | 2.12                     | 0.84              |
| 3:N:135:LEU:HD21  | 3:N:153:LEU:HB2   | 1.59                     | 0.84              |
| 3:N:819:GLY:CA    | 3:N:824:ASN:HD22  | 1.90                     | 0.84              |
| 5:P:101:GLU:HA    | 5:P:104:ARG:NH1   | 1.92                     | 0.84              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:406:ASP:HB2   | 3:D:424:GLY:N     | 1.91                     | 0.84              |
| 5:F:87:GLU:O      | 5:F:90:GLN:HB2    | 1.77                     | 0.84              |
| 2:M:373:VAL:HG12  | 2:M:374:ASN:H     | 1.41                     | 0.84              |
| 3:N:137:PRO:HG2   | 3:N:138:LYS:H     | 1.40                     | 0.84              |
| 1:B:137:ARG:NH1   | 1:B:139:ASN:HB2   | 1.91                     | 0.84              |
| 2:C:370:ALA:HA    | 2:C:373:VAL:HG23  | 1.60                     | 0.84              |
| 2:C:535:SER:O     | 2:C:538:GLN:HG2   | 1.76                     | 0.84              |
| 3:D:57:GLU:HG3    | 3:D:64:LYS:HA     | 1.59                     | 0.84              |
| 2:M:1092:LEU:HA   | 2:M:1095:LEU:HD12 | 1.58                     | 0.84              |
| 3:N:1494:ALA:CA   | 3:N:1497:GLU:HG2  | 2.04                     | 0.84              |
| 5:P:373:LYS:NZ    | 5:P:373:LYS:HB3   | 1.90                     | 0.84              |
| 2:C:233:GLU:CD    | 2:C:234:ALA:H     | 1.80                     | 0.84              |
| 2:C:71:TYR:H      | 2:C:71:TYR:HD2    | 1.26                     | 0.84              |
| 1:K:111:ALA:HA    | 1:K:129:ILE:HD11  | 1.59                     | 0.84              |
| 2:M:535:SER:O     | 2:M:538:GLN:HG2   | 1.77                     | 0.84              |
| 2:M:881:ASN:H     | 2:M:881:ASN:HD22  | 1.20                     | 0.84              |
| 2:C:193:LEU:HD12  | 2:C:196:LEU:HD12  | 1.57                     | 0.84              |
| 1:K:100:LEU:HB3   | 1:K:115:LEU:HD12  | 1.57                     | 0.84              |
| 2:M:194:VAL:HA    | 2:M:197:LEU:CG    | 2.07                     | 0.84              |
| 3:N:133:ILE:H     | 3:N:133:ILE:HD13  | 1.42                     | 0.84              |
| 3:N:562:ALA:HB3   | 3:N:567:ILE:HD11  | 1.59                     | 0.84              |
| 3:N:771:SER:HB2   | 3:N:778:LEU:HD22  | 1.60                     | 0.84              |
| 2:C:186:VAL:CG2   | 2:C:187:ASN:H     | 1.89                     | 0.84              |
| 2:C:643:VAL:HG23  | 2:C:647:GLN:NE2   | 1.93                     | 0.84              |
| 2:M:41:ASN:HD22   | 2:M:41:ASN:C      | 1.81                     | 0.84              |
| 1:L:57:TYR:CE1    | 1:L:163:ASN:HB2   | 2.13                     | 0.83              |
| 2:M:175:GLU:HG2   | 2:M:176:VAL:N     | 1.93                     | 0.83              |
| 3:N:322:VAL:HG23  | 3:N:335:LEU:HD11  | 1.60                     | 0.83              |
| 3:N:510:GLU:O     | 3:N:513:ILE:HG22  | 1.78                     | 0.83              |
| 1:B:175:ARG:HG3   | 1:B:201:THR:O     | 1.78                     | 0.83              |
| 2:C:838:LYS:HG3   | 2:C:997:LEU:HB2   | 1.60                     | 0.83              |
| 3:D:569:ASN:O     | 3:D:572:ARG:HB3   | 1.79                     | 0.83              |
| 2:M:762:LYS:HG2   | 2:M:763:GLY:N     | 1.93                     | 0.83              |
| 3:N:1459:LEU:HD12 | 3:N:1470:ARG:HH11 | 1.42                     | 0.83              |
| 3:N:368:VAL:HB    | 3:N:377:VAL:CG2   | 2.07                     | 0.83              |
| 3:N:420:VAL:O     | 3:N:421:LEU:HD23  | 1.77                     | 0.83              |
| 3:N:141:ILE:HB    | 3:N:450:TYR:HD2   | 1.41                     | 0.83              |
| 1:B:108:GLU:HG3   | 1:B:131:THR:HG22  | 1.61                     | 0.83              |
| 2:C:44:ILE:HG23   | 2:C:344:PHE:HE1   | 1.40                     | 0.83              |
| 2:M:1102:LEU:N    | 3:N:5:VAL:HG13    | 1.94                     | 0.83              |
| 2:M:285:LEU:HG    | 2:M:286:SER:N     | 1.92                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:323:GLU:O    | 3:N:333:LEU:HA    | 1.78                     | 0.83              |
| 2:C:1100:GLN:HG3 | 2:C:1102:LEU:HD21 | 1.60                     | 0.83              |
| 2:C:175:GLU:O    | 2:C:176:VAL:HG13  | 1.79                     | 0.83              |
| 3:D:206:ARG:HB2  | 3:D:392:SER:O     | 1.78                     | 0.83              |
| 3:D:706:PRO:HB2  | 3:D:708:LEU:HD21  | 1.58                     | 0.83              |
| 3:N:295:GLY:HA2  | 3:N:302:GLN:HB3   | 1.59                     | 0.83              |
| 3:N:543:LEU:O    | 3:N:546:ARG:HG3   | 1.77                     | 0.83              |
| 1:B:9:PRO:HG3    | 1:B:27:PRO:O      | 1.79                     | 0.83              |
| 2:C:881:ASN:N    | 2:C:881:ASN:HD22  | 1.73                     | 0.83              |
| 2:M:1100:GLN:HG3 | 2:M:1102:LEU:HD21 | 1.60                     | 0.83              |
| 3:N:119:SER:H    | 3:N:123:LEU:HG    | 1.43                     | 0.83              |
| 3:N:882:PHE:HA   | 3:N:885:ILE:HD12  | 1.60                     | 0.83              |
| 1:L:179:PHE:HB3  | 1:L:197:LEU:HD13  | 1.61                     | 0.83              |
| 2:M:91:GLN:HB2   | 2:M:118:ILE:O     | 1.78                     | 0.83              |
| 2:M:334:ARG:HA   | 2:M:338:GLU:OE1   | 1.77                     | 0.83              |
| 3:N:1147:ARG:HB2 | 3:N:1166:LEU:HD12 | 1.60                     | 0.83              |
| 1:B:185:ARG:HH22 | 3:D:692:GLU:HG3   | 1.41                     | 0.83              |
| 3:D:820:GLU:HG2  | 3:D:825:ALA:O     | 1.79                     | 0.83              |
| 2:M:631:SER:HB3  | 2:M:635:THR:H     | 1.42                     | 0.83              |
| 3:N:167:GLU:O    | 3:N:394:LEU:HD12  | 1.77                     | 0.83              |
| 3:D:209:ARG:O    | 3:D:346:ARG:HA    | 1.79                     | 0.83              |
| 3:N:192:ALA:HB3  | 3:N:195:VAL:HG23  | 1.60                     | 0.83              |
| 3:N:407:VAL:HG22 | 3:N:408:GLU:N     | 1.92                     | 0.83              |
| 5:P:305:GLU:HG3  | 5:P:309:LYS:HE3   | 1.59                     | 0.83              |
| 3:N:207:PHE:O    | 3:N:390:PRO:HA    | 1.78                     | 0.83              |
| 5:P:329:TYR:CD1  | 5:P:333:ILE:HD11  | 2.14                     | 0.83              |
| 2:C:266:ARG:HD2  | 2:C:273:GLY:H     | 1.43                     | 0.82              |
| 3:D:259:VAL:HG11 | 3:D:293:VAL:HA    | 1.61                     | 0.82              |
| 3:D:565:ILE:HG12 | 3:D:566:ILE:N     | 1.92                     | 0.82              |
| 3:N:124:GLU:HG3  | 3:N:128:TYR:CE2   | 2.13                     | 0.82              |
| 3:N:675:ARG:HH22 | 5:P:420:ASP:CB    | 1.92                     | 0.82              |
| 2:C:197:LEU:HD11 | 2:C:221:LEU:HD11  | 1.61                     | 0.82              |
| 3:D:408:GLU:HG3  | 3:D:421:LEU:C     | 2.00                     | 0.82              |
| 5:F:171:LYS:O    | 5:F:174:LEU:HB3   | 1.80                     | 0.82              |
| 3:N:1069:GLU:HA  | 3:N:1072:ILE:HD12 | 1.60                     | 0.82              |
| 1:A:5:LYS:NZ     | 1:A:192:LEU:HD22  | 1.93                     | 0.82              |
| 2:C:755:LEU:HD21 | 2:C:792:VAL:HG22  | 1.61                     | 0.82              |
| 3:D:317:VAL:HG23 | 3:D:338:GLU:O     | 1.79                     | 0.82              |
| 5:F:207:LEU:HB3  | 5:F:212:LEU:HD21  | 1.60                     | 0.82              |
| 1:A:14:ARG:HD2   | 1:B:234:ALA:N     | 1.94                     | 0.82              |
| 3:D:142:LEU:HB3  | 3:D:146:PRO:HA    | 1.58                     | 0.82              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:575:GLN:O     | 3:D:578:VAL:HB    | 1.78                     | 0.82              |
| 3:N:1399:ASP:O    | 3:N:1403:LEU:HB2  | 1.80                     | 0.82              |
| 3:N:154:THR:HG22  | 3:N:157:GLU:CG    | 2.08                     | 0.82              |
| 5:P:280:GLN:HG3   | 5:P:281:GLU:H     | 1.45                     | 0.82              |
| 5:P:418:LEU:HD12  | 5:P:418:LEU:N     | 1.93                     | 0.82              |
| 2:C:517:ARG:HB2   | 2:C:520:GLU:HB2   | 1.61                     | 0.82              |
| 3:D:119:SER:H     | 3:D:123:LEU:HD12  | 1.44                     | 0.82              |
| 3:D:1372:VAL:HA   | 3:D:1375:MET:HE3  | 1.61                     | 0.82              |
| 3:D:1388:ARG:NH2  | 3:D:1390:LEU:HD23 | 1.94                     | 0.82              |
| 3:D:1378:TYR:HB2  | 3:D:1422:MET:HE3  | 1.61                     | 0.82              |
| 1:K:42:ARG:NH1    | 1:L:34:VAL:HB     | 1.95                     | 0.82              |
| 1:L:212:ASN:O     | 1:L:215:VAL:HG22  | 1.80                     | 0.82              |
| 1:L:91:ASN:HB3    | 1:L:94:LEU:HG     | 1.61                     | 0.82              |
| 3:D:147:VAL:HG22  | 3:D:148:GLU:N     | 1.94                     | 0.82              |
| 3:D:207:PHE:O     | 3:D:390:PRO:HA    | 1.79                     | 0.82              |
| 3:D:353:VAL:CA    | 3:D:368:VAL:HG22  | 2.06                     | 0.82              |
| 1:K:102:LYS:HG2   | 1:K:139:ASN:OD1   | 1.79                     | 0.82              |
| 2:M:609:ASN:O     | 2:M:625:LEU:HB3   | 1.80                     | 0.82              |
| 3:N:16:GLU:H      | 3:N:16:GLU:CD     | 1.83                     | 0.82              |
| 3:D:1094:LEU:HD23 | 3:D:1230:GLY:HA2  | 1.62                     | 0.82              |
| 3:D:884:ARG:O     | 3:D:888:GLU:HG2   | 1.78                     | 0.82              |
| 2:C:1102:LEU:HD11 | 3:D:9:ARG:HD2     | 1.62                     | 0.82              |
| 5:F:413:SER:HB3   | 5:F:414:ARG:HH21  | 1.43                     | 0.82              |
| 3:N:1176:LYS:HA   | 3:N:1179:GLU:OE1  | 1.80                     | 0.82              |
| 2:C:477:GLY:HA2   | 2:C:508:ILE:HD12  | 1.61                     | 0.82              |
| 2:C:52:PHE:CD2    | 2:C:68:PHE:HB2    | 2.15                     | 0.82              |
| 3:D:1238:MET:HE2  | 3:D:1239:ARG:HB3  | 1.59                     | 0.82              |
| 3:D:295:GLY:HA2   | 3:D:302:GLN:CB    | 2.10                     | 0.82              |
| 3:D:355:VAL:CG1   | 3:D:385:VAL:HG21  | 2.08                     | 0.82              |
| 3:N:60:CYS:HB2    | 3:N:62:LYS:HE2    | 1.61                     | 0.82              |
| 3:N:658:LEU:HA    | 3:N:661:MET:HE3   | 1.61                     | 0.82              |
| 2:C:227:PHE:HA    | 2:C:237:ARG:HH12  | 1.43                     | 0.82              |
| 3:D:1397:LYS:HB2  | 3:D:1398:TRP:CZ3  | 2.15                     | 0.82              |
| 5:F:278:LEU:CB    | 5:F:286:PRO:HG3   | 2.10                     | 0.82              |
| 3:N:772:PRO:HG3   | 3:N:1210:SER:HB3  | 1.62                     | 0.82              |
| 5:P:102:LEU:CD1   | 5:P:183:ALA:HB1   | 2.09                     | 0.82              |
| 2:C:1085:PHE:O    | 2:C:1088:LEU:HB3  | 1.80                     | 0.82              |
| 2:M:328:LEU:HD12  | 2:M:437:ARG:HD2   | 1.61                     | 0.82              |
| 2:M:809:GLY:C     | 2:M:811:PRO:HD2   | 1.98                     | 0.82              |
| 2:C:1012:PRO:HD3  | 2:C:1026:GLN:HG2  | 1.62                     | 0.81              |
| 3:D:1231:GLU:HB3  | 3:D:1232:PRO:HD3  | 1.61                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:241:ILE:HA   | 3:D:312:ARG:HA    | 1.62                     | 0.81              |
| 2:M:194:VAL:HG22 | 2:M:221:LEU:HG    | 1.59                     | 0.81              |
| 2:M:51:THR:HG21  | 2:M:348:LEU:HG    | 1.59                     | 0.81              |
| 5:P:353:GLU:O    | 5:P:356:LYS:HB2   | 1.79                     | 0.81              |
| 2:C:166:PRO:CG   | 2:C:169:GLY:HA3   | 2.10                     | 0.81              |
| 2:C:841:ASN:ND2  | 2:C:845:ASN:HB3   | 1.95                     | 0.81              |
| 3:D:1213:ARG:HB2 | 3:D:1214:PRO:HD2  | 1.62                     | 0.81              |
| 3:D:806:PHE:CG   | 3:D:809:PRO:HB2   | 2.15                     | 0.81              |
| 2:M:1037:VAL:O   | 2:M:1041:GLU:HG3  | 1.79                     | 0.81              |
| 3:N:1472:ILE:CG2 | 3:N:1474:ALA:H    | 1.92                     | 0.81              |
| 3:N:433:GLY:HA3  | 3:N:447:VAL:O     | 1.80                     | 0.81              |
| 3:N:127:LEU:HD22 | 3:N:461:ILE:HD11  | 1.60                     | 0.81              |
| 5:P:368:VAL:HG23 | 5:P:369:LEU:N     | 1.94                     | 0.81              |
| 3:N:207:PHE:CZ   | 5:P:98:GLU:HG3    | 2.14                     | 0.81              |
| 1:B:138:LEU:HD12 | 1:B:139:ASN:H     | 1.46                     | 0.81              |
| 3:D:135:LEU:HD23 | 3:D:135:LEU:N     | 1.95                     | 0.81              |
| 3:D:264:LEU:HD22 | 3:D:316:GLN:NE2   | 1.96                     | 0.81              |
| 1:K:100:LEU:HD23 | 1:K:101:LEU:H     | 1.44                     | 0.81              |
| 3:N:141:ILE:HB   | 3:N:450:TYR:CD2   | 2.15                     | 0.81              |
| 3:N:252:ARG:HE   | 3:N:300:LYS:HA    | 1.44                     | 0.81              |
| 3:N:292:VAL:HG23 | 3:N:293:VAL:H     | 1.45                     | 0.81              |
| 3:N:458:ALA:HB1  | 3:N:513:ILE:HD11  | 1.60                     | 0.81              |
| 3:D:149:LYS:HE3  | 3:D:150:ARG:HE    | 1.43                     | 0.81              |
| 5:F:371:LEU:HA   | 5:F:375:LEU:HG    | 1.62                     | 0.81              |
| 2:M:322:VAL:HG12 | 2:M:323:ASP:H     | 1.45                     | 0.81              |
| 3:N:610:LYS:HZ1  | 3:N:1442:ASN:H    | 1.26                     | 0.81              |
| 5:P:274:THR:O    | 5:P:278:LEU:HG    | 1.79                     | 0.81              |
| 5:P:418:LEU:CD1  | 5:P:418:LEU:H     | 1.85                     | 0.81              |
| 2:C:958:THR:HG23 | 2:C:961:GLU:HB3   | 1.63                     | 0.81              |
| 3:N:402:PRO:HG3  | 3:N:443:VAL:HG22  | 1.61                     | 0.81              |
| 3:N:494:LYS:HA   | 3:N:1388:ARG:HH12 | 1.45                     | 0.81              |
| 3:N:820:GLU:HG2  | 3:N:825:ALA:O     | 1.81                     | 0.81              |
| 2:C:542:VAL:HG23 | 2:C:543:ASN:N     | 1.94                     | 0.81              |
| 3:D:225:LEU:HB3  | 3:D:226:PRO:CD    | 2.11                     | 0.81              |
| 1:L:206:THR:HB   | 1:L:209:GLU:CG    | 2.09                     | 0.81              |
| 2:M:230:ARG:HG2  | 2:M:233:GLU:HG3   | 1.62                     | 0.81              |
| 2:M:397:GLU:N    | 2:M:633:GLN:HE21  | 1.78                     | 0.81              |
| 5:P:370:LYS:HG3  | 5:P:371:LEU:N     | 1.94                     | 0.81              |
| 5:P:402:ASN:HB3  | 5:P:406:ARG:CZ    | 2.10                     | 0.81              |
| 2:C:194:VAL:HA   | 2:C:197:LEU:HG    | 1.61                     | 0.81              |
| 2:C:115:LEU:HB2  | 2:C:375:SER:HB3   | 1.62                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1495:ILE:HG13 | 4:E:84:ARG:NH1    | 1.95                     | 0.81              |
| 3:D:525:ARG:N     | 3:D:526:PRO:HD3   | 1.95                     | 0.81              |
| 2:M:164:PRO:HD3   | 2:M:266:ARG:NH2   | 1.94                     | 0.81              |
| 3:N:1152:GLU:N    | 3:N:1162:GLU:HB3  | 1.96                     | 0.81              |
| 3:N:119:SER:HB3   | 3:N:123:LEU:H     | 1.45                     | 0.81              |
| 1:A:78:ILE:O      | 1:A:81:ASN:HB2    | 1.81                     | 0.81              |
| 2:C:69:LEU:HD23   | 2:C:70:GLU:HG3    | 1.62                     | 0.81              |
| 3:D:30:GLU:CB     | 3:D:40:GLU:HG2    | 2.09                     | 0.81              |
| 2:M:170:PRO:HD3   | 2:M:263:ASP:HB3   | 1.61                     | 0.81              |
| 3:N:1372:VAL:HA   | 3:N:1375:MET:CE   | 2.10                     | 0.81              |
| 1:A:90:LEU:HD12   | 1:A:119:ASP:HA    | 1.61                     | 0.81              |
| 2:C:101:ILE:HG22  | 2:C:102:HIS:N     | 1.95                     | 0.81              |
| 2:C:149:THR:HG23  | 2:C:159:ILE:HG13  | 1.63                     | 0.81              |
| 2:C:876:VAL:H     | 2:C:877:PRO:HD2   | 1.45                     | 0.81              |
| 3:D:1311:LEU:HD12 | 3:D:1312:LEU:H    | 1.46                     | 0.81              |
| 3:N:1130:ARG:HH22 | 3:N:1323:GLN:HE22 | 1.27                     | 0.81              |
| 3:N:133:ILE:HG23  | 3:N:456:MET:CE    | 2.11                     | 0.81              |
| 3:N:642:CYS:SG    | 3:N:716:PHE:HB2   | 2.21                     | 0.81              |
| 5:P:282:LEU:HG    | 5:P:284:ARG:HG2   | 1.63                     | 0.81              |
| 5:P:417:LYS:HB2   | 5:P:418:LEU:HD12  | 1.62                     | 0.81              |
| 3:D:411:THR:HA    | 3:D:435:VAL:HG12  | 1.62                     | 0.81              |
| 2:M:198:ARG:HH21  | 2:M:231:PRO:HD3   | 1.46                     | 0.81              |
| 2:M:774:LEU:HA    | 2:M:777:ILE:HD12  | 1.62                     | 0.81              |
| 3:N:483:HIS:HB2   | 3:N:484:PRO:HD2   | 1.61                     | 0.81              |
| 2:C:226:VAL:HG23  | 2:C:227:PHE:HD1   | 1.46                     | 0.81              |
| 3:D:1151:ARG:C    | 3:D:1162:GLU:HB3  | 2.01                     | 0.81              |
| 3:D:387:LEU:N     | 3:D:387:LEU:HD12  | 1.96                     | 0.81              |
| 3:D:988:ARG:HG2   | 3:D:992:ILE:HD11  | 1.62                     | 0.81              |
| 3:N:1267:ARG:HH21 | 3:N:1271:LYS:NZ   | 1.78                     | 0.81              |
| 3:N:796:ARG:HE    | 3:N:861:GLN:HB2   | 1.45                     | 0.81              |
| 2:C:21:ILE:H      | 2:C:21:ILE:CD1    | 1.93                     | 0.80              |
| 2:C:689:VAL:CG2   | 2:C:870:ILE:HB    | 2.10                     | 0.80              |
| 2:C:810:ASP:N     | 2:C:811:PRO:HD2   | 1.96                     | 0.80              |
| 3:D:562:ALA:HB3   | 3:D:567:ILE:HD11  | 1.63                     | 0.80              |
| 5:P:152:ASP:O     | 5:P:156:VAL:HG21  | 1.82                     | 0.80              |
| 5:P:288:TYR:O     | 5:P:291:ILE:HG23  | 1.81                     | 0.80              |
| 2:C:347:GLY:HA2   | 2:C:350:ARG:HD2   | 1.63                     | 0.80              |
| 2:C:626:ARG:HG3   | 2:C:629:TYR:CD1   | 2.17                     | 0.80              |
| 3:D:678:GLU:HG3   | 3:D:679:ARG:HG3   | 1.62                     | 0.80              |
| 3:N:433:GLY:HA2   | 3:N:449:SER:N     | 1.97                     | 0.80              |
| 3:N:458:ALA:CB    | 3:N:513:ILE:HD11  | 2.11                     | 0.80              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:217:ASN:O     | 5:P:220:LEU:HB3   | 1.81                     | 0.80              |
| 2:C:346:VAL:HG23  | 2:C:347:GLY:H     | 1.46                     | 0.80              |
| 2:C:632:ASN:HB3   | 2:C:633:GLN:NE2   | 1.96                     | 0.80              |
| 2:C:666:LEU:HD11  | 2:C:668:LEU:HG    | 1.63                     | 0.80              |
| 3:D:644:LEU:HD12  | 3:D:645:PRO:HD2   | 1.61                     | 0.80              |
| 1:K:12:THR:HG22   | 1:L:229:GLN:HG2   | 1.63                     | 0.80              |
| 2:M:23:VAL:HG23   | 2:M:24:GLU:H      | 1.46                     | 0.80              |
| 2:C:162:ILE:HD12  | 2:C:172:ILE:HD12  | 1.64                     | 0.80              |
| 2:C:492:ASP:HB3   | 2:C:518:LYS:HE3   | 1.62                     | 0.80              |
| 3:D:113:GLY:C     | 3:D:115:LEU:H     | 1.83                     | 0.80              |
| 2:M:631:SER:HB3   | 2:M:635:THR:N     | 1.95                     | 0.80              |
| 1:A:151:VAL:HB    | 1:A:169:ALA:HB3   | 1.62                     | 0.80              |
| 2:C:801:VAL:HG22  | 2:C:826:TYR:O     | 1.81                     | 0.80              |
| 3:D:1018:ASN:O    | 3:D:1022:VAL:HG23 | 1.80                     | 0.80              |
| 3:D:1031:ASN:H    | 3:D:1034:GLN:HE21 | 1.29                     | 0.80              |
| 5:F:378:GLY:HA3   | 5:F:381:HIS:CE1   | 2.15                     | 0.80              |
| 1:L:38:ASN:HB3    | 1:L:39:PRO:HD3    | 1.62                     | 0.80              |
| 2:M:904:PRO:HB2   | 2:M:907:ASP:HB3   | 1.63                     | 0.80              |
| 3:N:1048:PRO:HG3  | 3:N:1075:HIS:HD2  | 1.45                     | 0.80              |
| 3:N:1490:LYS:HD2  | 4:O:39:VAL:HG13   | 1.63                     | 0.80              |
| 3:N:25:GLU:OE1    | 3:N:27:GLU:HG2    | 1.81                     | 0.80              |
| 3:D:149:LYS:HG3   | 3:D:150:ARG:HG2   | 1.63                     | 0.80              |
| 3:D:272:LEU:HD12  | 3:D:282:TYR:HE1   | 1.47                     | 0.80              |
| 3:D:582:LEU:O     | 3:D:603:LEU:HB2   | 1.82                     | 0.80              |
| 1:K:86:VAL:HG12   | 1:K:124:ASN:HD21  | 1.46                     | 0.80              |
| 3:N:174:GLY:HA2   | 3:N:389:GLU:HG2   | 1.63                     | 0.80              |
| 3:N:408:GLU:HB3   | 3:N:422:ALA:CB    | 2.10                     | 0.80              |
| 3:N:847:ASP:O     | 3:N:851:LEU:HG    | 1.82                     | 0.80              |
| 4:O:7:ASP:HA      | 4:O:10:PHE:HD1    | 1.47                     | 0.80              |
| 2:M:772:ARG:NE    | 5:P:373:LYS:HG3   | 1.95                     | 0.80              |
| 3:D:245:LEU:N     | 3:D:309:GLY:HA2   | 1.95                     | 0.80              |
| 3:D:244:GLU:HA    | 3:D:309:GLY:O     | 1.82                     | 0.80              |
| 5:P:111:GLU:HG3   | 5:P:114:LYS:HZ2   | 1.46                     | 0.80              |
| 2:C:303:PHE:H     | 2:C:303:PHE:HD1   | 1.26                     | 0.80              |
| 5:F:278:LEU:HB2   | 5:F:286:PRO:HG3   | 1.64                     | 0.80              |
| 2:M:108:ILE:CB    | 2:M:368:THR:HG21  | 2.11                     | 0.80              |
| 2:M:415:PRO:HB2   | 2:M:418:LEU:HB2   | 1.64                     | 0.80              |
| 3:N:1381:VAL:HG13 | 3:N:1389:LEU:O    | 1.81                     | 0.80              |
| 3:N:238:PRO:HB3   | 3:N:317:VAL:O     | 1.81                     | 0.80              |
| 2:C:341:THR:O     | 2:C:344:PHE:HB3   | 1.82                     | 0.80              |
| 3:D:1264:GLU:OE1  | 3:D:1423:GLY:HA3  | 1.81                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:128:TYR:HA    | 3:D:457:GLY:HA2  | 1.64                     | 0.80              |
| 5:F:81:VAL:HG23   | 5:F:82:ARG:N     | 1.96                     | 0.80              |
| 3:N:153:LEU:HD11  | 3:N:157:GLU:HB3  | 1.64                     | 0.80              |
| 3:N:261:LEU:HA    | 3:N:269:PHE:O    | 1.81                     | 0.80              |
| 3:N:268:ALA:HB3   | 3:N:290:PRO:HG3  | 1.63                     | 0.80              |
| 3:N:325:GLU:HG2   | 3:N:332:TYR:HB3  | 1.62                     | 0.80              |
| 3:N:141:ILE:HD12  | 3:N:450:TYR:HB3  | 1.63                     | 0.80              |
| 2:C:101:ILE:HG23  | 2:C:107:LEU:HD23 | 1.63                     | 0.80              |
| 2:C:274:ARG:HH21  | 2:C:284:ARG:HB3  | 1.47                     | 0.80              |
| 3:N:1486:VAL:HG22 | 4:O:75:PHE:CB    | 2.12                     | 0.80              |
| 3:N:445:ARG:H     | 3:N:445:ARG:HD2  | 1.47                     | 0.80              |
| 1:B:237:GLU:OE2   | 1:B:239:ALA:HB2  | 1.82                     | 0.79              |
| 1:B:97:VAL:HG12   | 1:B:98:THR:H     | 1.47                     | 0.79              |
| 2:C:101:ILE:HG22  | 2:C:102:HIS:H    | 1.46                     | 0.79              |
| 3:D:1083:ASP:HB2  | 3:D:1239:ARG:NH2 | 1.96                     | 0.79              |
| 3:D:33:ASN:HD21   | 3:D:35:ARG:CG    | 1.85                     | 0.79              |
| 1:K:45:LEU:HD21   | 1:K:177:VAL:HB   | 1.62                     | 0.79              |
| 3:N:1494:ALA:HA   | 3:N:1497:GLU:CG  | 2.07                     | 0.79              |
| 3:N:555:LYS:HA    | 3:N:558:LEU:HD12 | 1.61                     | 0.79              |
| 5:P:253:ASP:HA    | 5:P:259:ARG:NH1  | 1.97                     | 0.79              |
| 5:F:372:ARG:HG3   | 5:F:378:GLY:O    | 1.82                     | 0.79              |
| 1:L:28:LEU:HB3    | 1:L:193:ASP:HB2  | 1.61                     | 0.79              |
| 2:M:98:LEU:HD11   | 2:M:113:VAL:HG21 | 1.64                     | 0.79              |
| 2:M:23:VAL:HA     | 2:M:121:MET:HE1  | 1.64                     | 0.79              |
| 2:M:654:LEU:HD12  | 2:M:655:LEU:H    | 1.45                     | 0.79              |
| 3:N:400:VAL:HG23  | 3:N:443:VAL:HG13 | 1.62                     | 0.79              |
| 5:P:94:LEU:HG     | 5:P:190:ALA:HB1  | 1.64                     | 0.79              |
| 5:P:219:GLY:HA3   | 5:P:246:ALA:HB2  | 1.64                     | 0.79              |
| 2:C:230:ARG:HG2   | 2:C:233:GLU:CG   | 2.10                     | 0.79              |
| 5:F:270:LYS:HE3   | 5:F:295:MET:SD   | 2.22                     | 0.79              |
| 1:K:35:THR:O      | 1:K:39:PRO:HG2   | 1.83                     | 0.79              |
| 3:N:1170:ASP:O    | 3:N:1173:LEU:HB3 | 1.83                     | 0.79              |
| 2:C:290:LEU:CD2   | 2:C:302:VAL:HG21 | 2.12                     | 0.79              |
| 3:D:230:TRP:NE1   | 3:D:233:LYS:HG3  | 1.98                     | 0.79              |
| 3:D:25:GLU:HB2    | 3:D:92:HIS:CE1   | 2.16                     | 0.79              |
| 3:N:837:GLY:HA2   | 3:N:841:TYR:HD1  | 1.45                     | 0.79              |
| 2:C:197:LEU:HB3   | 2:C:207:LEU:HD13 | 1.64                     | 0.79              |
| 2:C:382:ILE:O     | 2:C:385:PHE:HB3  | 1.81                     | 0.79              |
| 3:D:207:PHE:HB2   | 3:D:391:ALA:HB3  | 1.64                     | 0.79              |
| 2:M:72:ARG:O      | 2:M:94:LEU:HD12  | 1.81                     | 0.79              |
| 3:N:158:TYR:CE1   | 3:N:454:ALA:HB3  | 2.17                     | 0.79              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:100:LEU:HD23  | 2:C:368:THR:CA   | 2.01                     | 0.79              |
| 2:C:571:LEU:HD22  | 2:C:701:THR:H    | 1.47                     | 0.79              |
| 3:D:1394:VAL:HB   | 3:D:1397:LYS:HE2 | 1.65                     | 0.79              |
| 3:D:154:THR:HG22  | 3:D:157:GLU:CG   | 2.12                     | 0.79              |
| 2:M:292:ARG:HG2   | 2:M:297:GLU:O    | 1.83                     | 0.79              |
| 3:N:441:ARG:HG3   | 3:N:443:VAL:CG2  | 2.13                     | 0.79              |
| 3:N:806:PHE:HA    | 3:N:809:PRO:CD   | 2.11                     | 0.79              |
| 3:D:1405:GLU:OE2  | 3:D:1407:LEU:HG  | 1.83                     | 0.79              |
| 3:D:1472:ILE:HD13 | 3:D:1473:PRO:HD2 | 1.65                     | 0.79              |
| 3:D:412:GLY:H     | 3:D:435:VAL:HB   | 1.47                     | 0.79              |
| 2:M:543:ASN:HA    | 2:M:546:LEU:HD12 | 1.64                     | 0.79              |
| 1:L:112:ARG:NH1   | 1:L:125:PRO:HB2  | 1.98                     | 0.79              |
| 2:M:165:LEU:O     | 2:M:165:LEU:HD23 | 1.83                     | 0.79              |
| 2:M:479:VAL:H     | 2:M:506:ASN:HB3  | 1.47                     | 0.79              |
| 2:M:72:ARG:CG     | 2:M:95:TYR:HB2   | 2.12                     | 0.79              |
| 3:N:147:VAL:CG2   | 3:N:148:GLU:H    | 1.94                     | 0.79              |
| 3:N:693:GLU:HA    | 4:O:48:MET:HE3   | 1.64                     | 0.79              |
| 5:P:333:ILE:N     | 5:P:333:ILE:HD12 | 1.97                     | 0.79              |
| 3:N:675:ARG:NH2   | 5:P:420:ASP:HB3  | 1.95                     | 0.79              |
| 1:A:15:THR:HB     | 1:A:21:GLY:HA3   | 1.65                     | 0.79              |
| 2:C:414:GLY:H     | 2:C:419:THR:HG21 | 1.47                     | 0.79              |
| 3:D:14:SER:HB2    | 3:D:17:LYS:H     | 1.48                     | 0.79              |
| 3:D:535:PHE:O     | 5:F:314:PRO:HB2  | 1.83                     | 0.79              |
| 5:F:396:ARG:HA    | 5:F:399:GLN:HE21 | 1.46                     | 0.79              |
| 3:N:387:LEU:H     | 3:N:387:LEU:HD12 | 1.48                     | 0.79              |
| 3:D:1232:PRO:O    | 3:D:1235:GLN:HG2 | 1.82                     | 0.79              |
| 3:D:655:PRO:HA    | 3:D:658:LEU:HD12 | 1.65                     | 0.79              |
| 3:D:799:LYS:HB3   | 3:D:800:LYS:CE   | 2.13                     | 0.79              |
| 1:L:219:ARG:HG2   | 1:L:219:ARG:HH11 | 1.48                     | 0.79              |
| 2:M:197:LEU:HB3   | 2:M:207:LEU:CD1  | 2.11                     | 0.79              |
| 3:N:227:LEU:HD11  | 3:N:327:GLU:H    | 1.47                     | 0.79              |
| 3:D:1183:ILE:HG13 | 3:D:1184:GLN:N   | 1.97                     | 0.78              |
| 3:D:1472:ILE:O    | 3:D:1477:GLY:HA3 | 1.82                     | 0.78              |
| 1:K:206:THR:HB    | 1:K:209:GLU:CG   | 2.12                     | 0.78              |
| 2:M:715:THR:HG22  | 2:M:717:LEU:H    | 1.48                     | 0.78              |
| 2:M:737:LEU:HA    | 2:M:743:VAL:HA   | 1.64                     | 0.78              |
| 2:C:47:ALA:HA     | 2:C:50:GLU:OE2   | 1.83                     | 0.78              |
| 2:C:720:GLU:HB3   | 2:C:760:SER:HB3  | 1.63                     | 0.78              |
| 3:D:1307:LYS:H    | 3:D:1307:LYS:CE  | 1.95                     | 0.78              |
| 3:D:658:LEU:HD23  | 3:D:661:MET:HE1  | 1.66                     | 0.78              |
| 3:D:82:LYS:HB2    | 3:D:84:ILE:HG22  | 1.65                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:676:MET:HG3   | 3:N:677:LEU:HD23 | 1.65                     | 0.78              |
| 2:C:1:MET:HB2     | 2:C:899:GLN:HA   | 1.65                     | 0.78              |
| 2:C:949:LYS:HZ2   | 3:D:796:ARG:HH12 | 1.32                     | 0.78              |
| 2:M:512:ARG:HD2   | 2:M:523:ILE:HG12 | 1.65                     | 0.78              |
| 3:D:162:ARG:NH1   | 3:D:434:ARG:HH22 | 1.82                     | 0.78              |
| 3:D:98:PRO:HA     | 3:D:514:LEU:O    | 1.83                     | 0.78              |
| 1:L:58:ILE:HG12   | 1:L:140:MET:HB3  | 1.65                     | 0.78              |
| 3:N:1486:VAL:HG22 | 4:O:75:PHE:HB3   | 1.65                     | 0.78              |
| 3:N:288:MET:CE    | 3:N:307:ALA:HB2  | 2.13                     | 0.78              |
| 3:N:416:ALA:CB    | 3:N:432:TYR:HA   | 2.08                     | 0.78              |
| 3:N:711:LEU:HB3   | 3:N:735:ALA:HB1  | 1.65                     | 0.78              |
| 3:N:841:TYR:HB2   | 3:N:864:VAL:HG13 | 1.64                     | 0.78              |
| 5:P:173:TYR:HA    | 5:P:176:ILE:HD12 | 1.63                     | 0.78              |
| 3:D:843:PHE:CE2   | 3:D:864:VAL:HG11 | 2.16                     | 0.78              |
| 3:D:537:THR:O     | 5:F:317:LEU:HG   | 1.82                     | 0.78              |
| 2:M:290:LEU:HD22  | 2:M:302:VAL:HG21 | 1.64                     | 0.78              |
| 2:M:773:LEU:HG    | 2:M:774:LEU:N    | 1.99                     | 0.78              |
| 3:N:433:GLY:CA    | 3:N:449:SER:H    | 1.96                     | 0.78              |
| 3:D:252:ARG:CZ    | 3:D:300:LYS:HG2  | 2.14                     | 0.78              |
| 5:F:234:LYS:HE2   | 5:F:236:SER:HB3  | 1.64                     | 0.78              |
| 2:M:265:ARG:HB2   | 2:M:267:TYR:O    | 1.84                     | 0.78              |
| 2:M:157:ARG:HD2   | 2:M:314:THR:HG22 | 1.63                     | 0.78              |
| 2:M:834:GLN:HG3   | 2:M:837:ASP:OD2  | 1.84                     | 0.78              |
| 3:N:875:THR:HG22  | 3:N:879:ARG:HG3  | 1.64                     | 0.78              |
| 1:B:13:VAL:HG22   | 1:B:14:ARG:H     | 1.49                     | 0.78              |
| 2:C:689:VAL:HG22  | 2:C:870:ILE:HB   | 1.66                     | 0.78              |
| 3:D:542:ASP:O     | 3:D:546:ARG:HG2  | 1.83                     | 0.78              |
| 3:D:799:LYS:HB3   | 3:D:800:LYS:HE3  | 1.66                     | 0.78              |
| 5:F:90:GLN:O      | 5:F:92:PRO:HD3   | 1.83                     | 0.78              |
| 2:M:208:ALA:HB2   | 2:M:221:LEU:HD22 | 1.63                     | 0.78              |
| 2:M:600:ASP:CB    | 2:M:650:ARG:HA   | 2.14                     | 0.78              |
| 2:M:755:LEU:HD21  | 2:M:792:VAL:HG22 | 1.66                     | 0.78              |
| 3:N:610:LYS:NZ    | 3:N:1442:ASN:H   | 1.80                     | 0.78              |
| 2:C:367:LEU:HG    | 2:C:372:LEU:HD21 | 1.64                     | 0.78              |
| 2:C:649:VAL:HA    | 2:C:650:ARG:HH21 | 1.49                     | 0.78              |
| 3:N:135:LEU:O     | 3:N:150:ARG:HA   | 1.84                     | 0.78              |
| 3:N:230:TRP:HE1   | 3:N:233:LYS:HG3  | 1.49                     | 0.78              |
| 2:M:1071:ILE:O    | 3:N:659:LYS:HD3  | 1.83                     | 0.78              |
| 5:P:209:PHE:CD2   | 5:P:213:ILE:HD11 | 2.18                     | 0.78              |
| 2:C:15:LEU:HD12   | 2:C:15:LEU:N     | 1.99                     | 0.78              |
| 3:D:1103:HIS:CD2  | 3:D:1463:LYS:H   | 2.01                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:49:GLN:HA     | 4:E:53:GLY:O      | 1.83                     | 0.78              |
| 3:N:238:PRO:HG3   | 3:N:318:ARG:HG2   | 1.66                     | 0.78              |
| 3:N:526:PRO:O     | 3:N:537:THR:HG22  | 1.84                     | 0.78              |
| 3:N:858:VAL:HG12  | 3:N:859:ASP:N     | 1.99                     | 0.78              |
| 5:P:264:MET:HA    | 5:P:264:MET:HE2   | 1.65                     | 0.78              |
| 5:P:353:GLU:HA    | 5:P:356:LYS:HD2   | 1.66                     | 0.78              |
| 1:L:111:ALA:HB3   | 1:L:125:PRO:HA    | 1.65                     | 0.78              |
| 1:L:241:GLU:N     | 1:L:242:PRO:HD2   | 1.99                     | 0.78              |
| 3:N:1267:ARG:CB   | 3:N:1267:ARG:HH11 | 1.97                     | 0.78              |
| 2:M:1031:ARG:HB2  | 3:N:622:ARG:HH12  | 1.48                     | 0.78              |
| 3:N:782:SER:H     | 3:N:785:ILE:HD12  | 1.48                     | 0.78              |
| 3:N:85:VAL:HG21   | 3:N:89:ARG:CZ     | 2.14                     | 0.78              |
| 3:D:225:LEU:HD11  | 3:D:242:LEU:HD11  | 1.64                     | 0.77              |
| 3:D:225:LEU:HD12  | 3:D:333:LEU:HD11  | 1.65                     | 0.77              |
| 3:D:417:PRO:HA    | 3:D:429:SER:O     | 1.83                     | 0.77              |
| 3:D:808:THR:H     | 3:D:809:PRO:HD2   | 1.50                     | 0.77              |
| 1:K:39:PRO:HG3    | 1:L:39:PRO:HG3    | 1.66                     | 0.77              |
| 2:C:606:VAL:HG12  | 2:C:611:ILE:HG23  | 1.66                     | 0.77              |
| 2:C:600:ASP:HB3   | 2:C:650:ARG:HA    | 1.66                     | 0.77              |
| 3:D:421:LEU:HD23  | 3:D:427:VAL:CG1   | 2.14                     | 0.77              |
| 4:E:76:GLY:HA3    | 4:E:79:LEU:HD21   | 1.65                     | 0.77              |
| 2:M:21:ILE:CD1    | 2:M:21:ILE:H      | 1.96                     | 0.77              |
| 2:C:91:GLN:HA     | 2:C:120:LEU:HG    | 1.65                     | 0.77              |
| 2:C:575:GLN:N     | 2:C:667:ALA:HB1   | 1.99                     | 0.77              |
| 3:D:1380:GLU:HG2  | 3:D:1381:VAL:H    | 1.48                     | 0.77              |
| 3:D:258:VAL:HB    | 3:D:273:ARG:CB    | 2.07                     | 0.77              |
| 3:D:36:THR:HB     | 3:D:38:LYS:HG2    | 1.65                     | 0.77              |
| 3:D:827:ILE:HA    | 3:D:836:VAL:HB    | 1.64                     | 0.77              |
| 3:D:989:TYR:HA    | 3:D:992:ILE:HD12  | 1.66                     | 0.77              |
| 1:L:78:ILE:HG22   | 1:L:82:LEU:HD21   | 1.66                     | 0.77              |
| 2:M:773:LEU:HD23  | 5:P:354:LEU:HD22  | 1.67                     | 0.77              |
| 2:M:837:ASP:O     | 2:M:849:VAL:HG23  | 1.83                     | 0.77              |
| 3:N:1286:THR:HG22 | 3:N:1288:GLU:N    | 1.95                     | 0.77              |
| 3:N:1496:GLU:HA   | 3:N:1499:ARG:HB3  | 1.67                     | 0.77              |
| 3:N:352:ASN:C     | 3:N:368:VAL:HG13  | 2.05                     | 0.77              |
| 1:B:13:VAL:HG22   | 1:B:14:ARG:N      | 1.99                     | 0.77              |
| 2:C:21:ILE:HD12   | 2:C:21:ILE:N      | 1.98                     | 0.77              |
| 2:C:266:ARG:HB2   | 2:C:272:ALA:HB3   | 1.65                     | 0.77              |
| 2:C:413:LEU:HA    | 2:C:419:THR:HG21  | 1.65                     | 0.77              |
| 3:D:804:LEU:O     | 3:D:805:GLU:HG2   | 1.83                     | 0.77              |
| 3:D:945:SER:OG    | 3:D:947:ILE:HG22  | 1.84                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:1102:LEU:H    | 3:N:5:VAL:HG13   | 1.48                     | 0.77              |
| 3:N:387:LEU:N     | 3:N:387:LEU:HD12 | 2.00                     | 0.77              |
| 3:N:407:VAL:CG2   | 3:N:408:GLU:H    | 1.96                     | 0.77              |
| 5:P:156:VAL:HG23  | 5:P:157:GLU:OE1  | 1.84                     | 0.77              |
| 1:A:211:LEU:O     | 1:A:215:VAL:HG23 | 1.85                     | 0.77              |
| 2:C:141:HIS:CE1   | 2:C:332:ARG:HB3  | 2.19                     | 0.77              |
| 2:C:605:LYS:HB3   | 2:C:610:ARG:HH21 | 1.48                     | 0.77              |
| 3:D:853:VAL:HG13  | 3:D:858:VAL:O    | 1.85                     | 0.77              |
| 5:F:350:LEU:HG    | 5:F:354:LEU:HD11 | 1.66                     | 0.77              |
| 5:F:368:VAL:HG23  | 5:F:369:LEU:N    | 2.00                     | 0.77              |
| 2:M:516:ARG:HA    | 2:M:520:GLU:O    | 1.84                     | 0.77              |
| 3:N:1048:PRO:HG3  | 3:N:1075:HIS:CD2 | 2.20                     | 0.77              |
| 3:N:241:ILE:HA    | 3:N:312:ARG:HA   | 1.64                     | 0.77              |
| 3:N:800:LYS:HD2   | 3:N:801:GLY:N    | 1.99                     | 0.77              |
| 4:O:40:LEU:HD13   | 4:O:72:ARG:HH12  | 1.49                     | 0.77              |
| 2:C:759:THR:HB    | 2:C:785:VAL:CG1  | 2.13                     | 0.77              |
| 3:D:841:TYR:HB2   | 3:D:864:VAL:HG13 | 1.65                     | 0.77              |
| 4:E:61:GLU:H      | 4:E:61:GLU:CD    | 1.87                     | 0.77              |
| 1:K:14:ARG:HD2    | 1:L:233:VAL:HA   | 1.64                     | 0.77              |
| 2:M:397:GLU:H     | 2:M:633:GLN:NE2  | 1.80                     | 0.77              |
| 3:N:433:GLY:HA2   | 3:N:449:SER:H    | 1.48                     | 0.77              |
| 3:N:476:GLU:O     | 3:N:479:GLU:HB2  | 1.84                     | 0.77              |
| 5:P:367:MET:HB2   | 5:P:371:LEU:CG   | 2.15                     | 0.77              |
| 1:B:153:ALA:HA    | 1:B:156:HIS:CE1  | 2.19                     | 0.77              |
| 3:D:1048:PRO:HG3  | 3:D:1075:HIS:HD2 | 1.48                     | 0.77              |
| 1:L:181:VAL:HG22  | 1:L:195:LEU:HD13 | 1.67                     | 0.77              |
| 3:N:921:ARG:NH1   | 3:N:921:ARG:HB3  | 1.99                     | 0.77              |
| 1:A:154:GLU:H     | 1:A:154:GLU:CD   | 1.88                     | 0.77              |
| 1:B:104:GLU:HA    | 1:B:132:LEU:HD13 | 1.66                     | 0.77              |
| 3:D:1380:GLU:HG2  | 3:D:1381:VAL:N   | 1.99                     | 0.77              |
| 2:M:325:ILE:N     | 2:M:325:ILE:HD12 | 1.98                     | 0.77              |
| 2:M:625:LEU:HD11  | 2:M:639:GLN:HB2  | 1.66                     | 0.77              |
| 3:N:297:ILE:HG12  | 3:N:298:VAL:HG23 | 1.67                     | 0.77              |
| 1:K:38:ASN:HB3    | 1:K:39:PRO:HD3   | 1.65                     | 0.77              |
| 2:M:74:GLY:O      | 2:M:76:PRO:HD3   | 1.84                     | 0.77              |
| 3:N:815:ALA:HA    | 3:N:818:ARG:HD2  | 1.67                     | 0.77              |
| 5:P:102:LEU:HD12  | 5:P:183:ALA:HB1  | 1.67                     | 0.77              |
| 1:A:86:VAL:HG12   | 1:A:124:ASN:ND2  | 2.00                     | 0.77              |
| 2:C:413:LEU:HA    | 2:C:419:THR:CG2  | 2.13                     | 0.77              |
| 3:D:1286:THR:HG22 | 3:D:1288:GLU:H   | 1.49                     | 0.77              |
| 1:K:86:VAL:HG13   | 1:K:123:MET:HB2  | 1.64                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:1051:GLU:HG3  | 2:M:1052:MET:N   | 1.99                     | 0.77              |
| 2:M:355:VAL:HA    | 2:M:358:ARG:HG3  | 1.67                     | 0.77              |
| 2:M:580:MET:HB3   | 2:M:584:GLU:OE2  | 1.84                     | 0.77              |
| 3:N:1472:ILE:HG23 | 3:N:1474:ALA:H   | 1.50                     | 0.77              |
| 3:N:490:ALA:HA    | 3:N:493:ARG:NE   | 2.00                     | 0.77              |
| 3:N:548:ILE:HG22  | 3:N:552:ASN:ND2  | 1.96                     | 0.77              |
| 3:N:734:GLU:OE1   | 3:N:734:GLU:HA   | 1.85                     | 0.77              |
| 5:P:333:ILE:HD12  | 5:P:333:ILE:H    | 1.48                     | 0.77              |
| 2:C:1051:GLU:HG3  | 2:C:1052:MET:N   | 1.98                     | 0.76              |
| 3:D:440:VAL:HG23  | 3:D:441:ARG:N    | 1.99                     | 0.76              |
| 3:N:761:ILE:HG22  | 3:N:762:GLN:N    | 1.98                     | 0.76              |
| 1:B:152:PRO:HG2   | 1:B:155:LYS:CB   | 2.16                     | 0.76              |
| 1:B:58:ILE:CG2    | 1:B:61:VAL:HB    | 2.15                     | 0.76              |
| 3:D:793:THR:HG21  | 3:D:906:GLN:HG2  | 1.68                     | 0.76              |
| 1:K:224:TYR:CE1   | 1:L:9:PRO:HD2    | 2.19                     | 0.76              |
| 2:M:93:PRO:CA     | 2:M:117:HIS:HB3  | 2.15                     | 0.76              |
| 2:M:194:VAL:CA    | 2:M:197:LEU:HG   | 2.13                     | 0.76              |
| 2:M:193:LEU:HG    | 2:M:197:LEU:HD21 | 1.67                     | 0.76              |
| 3:N:1041:LEU:CD1  | 3:N:1058:ARG:HA  | 2.15                     | 0.76              |
| 3:N:119:SER:HB3   | 3:N:123:LEU:HG   | 1.67                     | 0.76              |
| 3:N:1380:GLU:HG2  | 3:N:1381:VAL:H   | 1.48                     | 0.76              |
| 3:N:612:GLY:O     | 3:N:615:ARG:HG2  | 1.85                     | 0.76              |
| 3:N:646:LYS:HG2   | 3:N:720:LEU:HB3  | 1.66                     | 0.76              |
| 4:O:7:ASP:HA      | 4:O:10:PHE:CD1   | 2.20                     | 0.76              |
| 2:M:780:GLU:HG2   | 5:P:379:ARG:NH2  | 2.00                     | 0.76              |
| 2:C:100:LEU:HD21  | 2:C:367:LEU:HD23 | 1.67                     | 0.76              |
| 2:C:184:MET:HG3   | 2:C:193:LEU:HD13 | 1.66                     | 0.76              |
| 2:C:264:PRO:HB2   | 2:C:289:THR:HG21 | 1.66                     | 0.76              |
| 3:D:140:ALA:N     | 3:D:450:TYR:CE2  | 2.52                     | 0.76              |
| 3:D:654:LYS:HB3   | 3:D:655:PRO:HD3  | 1.65                     | 0.76              |
| 2:M:37:GLU:HG2    | 2:M:71:TYR:CE2   | 2.20                     | 0.76              |
| 3:N:1253:THR:HG22 | 3:N:1254:GLN:H   | 1.46                     | 0.76              |
| 3:N:160:GLU:CD    | 3:N:165:LYS:HE2  | 2.06                     | 0.76              |
| 3:N:367:ILE:HB    | 3:N:377:VAL:CG1  | 2.14                     | 0.76              |
| 1:A:152:PRO:HG2   | 1:A:155:LYS:HB2  | 1.67                     | 0.76              |
| 1:B:206:THR:HB    | 1:B:209:GLU:CG   | 2.13                     | 0.76              |
| 2:C:309:TYR:CE2   | 2:C:321:GLU:HG3  | 2.20                     | 0.76              |
| 2:C:631:SER:HB3   | 2:C:635:THR:N    | 2.00                     | 0.76              |
| 3:D:1213:ARG:HH11 | 3:D:1213:ARG:HG2 | 1.50                     | 0.76              |
| 3:D:253:ALA:N     | 3:D:301:GLY:HA3  | 2.00                     | 0.76              |
| 5:F:156:VAL:HG23  | 5:F:157:GLU:H    | 1.49                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:353:GLU:O     | 5:F:356:LYS:HB2   | 1.84                     | 0.76              |
| 2:M:101:ILE:HG22  | 2:M:102:HIS:N     | 2.01                     | 0.76              |
| 3:N:119:SER:H     | 3:N:123:LEU:HB2   | 1.50                     | 0.76              |
| 3:N:253:ALA:N     | 3:N:301:GLY:HA3   | 1.99                     | 0.76              |
| 3:N:421:LEU:HG    | 3:N:428:LYS:CA    | 2.10                     | 0.76              |
| 3:N:671:LYS:HA    | 3:N:674:ARG:HB2   | 1.64                     | 0.76              |
| 1:B:32:PHE:HA     | 1:B:35:THR:CB     | 2.14                     | 0.76              |
| 2:C:468:ARG:HA    | 2:C:486:MET:O     | 1.85                     | 0.76              |
| 2:C:988:VAL:HG12  | 3:D:948:THR:CB    | 2.14                     | 0.76              |
| 3:D:1345:GLU:O    | 3:D:1349:VAL:HG23 | 1.85                     | 0.76              |
| 4:E:46:PRO:HB2    | 4:E:57:ASP:HB3    | 1.66                     | 0.76              |
| 3:N:1095:THR:HG23 | 3:N:1230:GLY:HA3  | 1.66                     | 0.76              |
| 3:N:219:GLU:O     | 3:N:337:LEU:HG    | 1.84                     | 0.76              |
| 2:M:1100:GLN:O    | 3:N:8:VAL:HA      | 1.85                     | 0.76              |
| 3:D:1114:THR:HB   | 3:D:1195:GLN:HG3  | 1.68                     | 0.76              |
| 5:F:276:ARG:O     | 5:F:280:GLN:HG2   | 1.85                     | 0.76              |
| 5:F:353:GLU:HG3   | 5:F:356:LYS:HD2   | 1.67                     | 0.76              |
| 2:M:385:PHE:CD1   | 2:M:389:SER:HB2   | 2.21                     | 0.76              |
| 2:M:428:ARG:NE    | 2:M:451:LEU:HD21  | 2.01                     | 0.76              |
| 2:C:167:LYS:HE2   | 2:C:168:ARG:HE    | 1.50                     | 0.76              |
| 2:C:17:PRO:HB2    | 2:C:20:GLU:HB2    | 1.68                     | 0.76              |
| 3:D:1216:SER:HB2  | 4:E:15:SER:HA     | 1.68                     | 0.76              |
| 3:D:119:SER:HB3   | 3:D:123:LEU:HG    | 1.66                     | 0.76              |
| 3:D:1099:VAL:HG12 | 10:D:1529:NE6:C14 | 2.16                     | 0.76              |
| 3:D:361:VAL:CG1   | 3:D:379:ALA:HB1   | 2.16                     | 0.76              |
| 5:F:380:GLU:HA    | 5:F:385:GLU:OE1   | 1.84                     | 0.76              |
| 3:N:1213:ARG:HB2  | 3:N:1214:PRO:HD2  | 1.67                     | 0.76              |
| 3:N:165:LYS:O     | 3:N:396:VAL:HA    | 1.84                     | 0.76              |
| 3:N:285:PRO:HB3   | 3:N:313:MET:SD    | 2.25                     | 0.76              |
| 2:C:1064:ASN:HA   | 5:F:341:PRO:CB    | 2.15                     | 0.76              |
| 2:C:958:THR:HG23  | 2:C:961:GLU:CB    | 2.15                     | 0.76              |
| 3:D:322:VAL:HA    | 3:D:335:LEU:HG    | 1.66                     | 0.76              |
| 3:D:801:GLY:HA2   | 3:D:830:ALA:O     | 1.86                     | 0.76              |
| 4:E:6:ILE:HG13    | 4:E:10:PHE:CE1    | 2.20                     | 0.76              |
| 5:F:261:PRO:HD2   | 5:F:264:MET:HG3   | 1.66                     | 0.76              |
| 5:F:302:LYS:HD2   | 5:F:303:ARG:N     | 2.00                     | 0.76              |
| 1:L:150:TYR:OH    | 1:L:168:ASP:HB3   | 1.85                     | 0.76              |
| 1:L:176:ARG:HG2   | 1:L:177:VAL:N     | 2.01                     | 0.76              |
| 1:L:18:ARG:HH12   | 1:L:88:ARG:HH22   | 1.30                     | 0.76              |
| 3:N:553:ARG:NH1   | 5:P:214:GLN:HB2   | 2.00                     | 0.76              |
| 2:C:226:VAL:HG23  | 2:C:227:PHE:CD1   | 2.20                     | 0.76              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:285:LEU:HG    | 2:C:286:SER:N     | 2.00                     | 0.76              |
| 2:C:84:ARG:HA     | 2:C:131:GLY:HA2   | 1.68                     | 0.76              |
| 3:D:1211:MET:HB2  | 3:D:1213:ARG:HH11 | 1.51                     | 0.76              |
| 3:D:1398:TRP:N    | 3:D:1398:TRP:HE3  | 1.84                     | 0.76              |
| 3:D:1480:PHE:CD2  | 3:D:1481:VAL:HG23 | 2.20                     | 0.76              |
| 3:D:65:ARG:CG     | 3:D:67:ARG:HG2    | 2.16                     | 0.76              |
| 3:D:875:THR:HG22  | 3:D:876:SER:H     | 1.51                     | 0.76              |
| 3:D:931:LEU:CA    | 3:D:934:LEU:HD12  | 2.13                     | 0.76              |
| 3:D:960:LYS:HE3   | 3:D:964:LEU:HD11  | 1.67                     | 0.76              |
| 3:N:1119:SER:HA   | 3:N:1186:VAL:O    | 1.86                     | 0.76              |
| 3:N:409:VAL:HG12  | 3:N:413:ASP:OD2   | 1.84                     | 0.76              |
| 5:P:242:TRP:HA    | 5:P:245:GLN:HG2   | 1.66                     | 0.76              |
| 1:A:228:PRO:O     | 1:A:229:GLN:HG3   | 1.85                     | 0.76              |
| 1:B:112:ARG:HH12  | 1:B:125:PRO:HB2   | 1.49                     | 0.76              |
| 1:B:104:GLU:HB3   | 1:B:137:ARG:CG    | 2.13                     | 0.76              |
| 3:D:191:LEU:HD23  | 3:D:195:VAL:HG11  | 1.67                     | 0.76              |
| 3:D:992:ILE:O     | 3:D:995:LEU:HB3   | 1.85                     | 0.76              |
| 5:F:113:ILE:HD13  | 5:F:128:ARG:HB3   | 1.66                     | 0.76              |
| 2:C:1067:TYR:CE2  | 5:F:342:VAL:HA    | 2.21                     | 0.76              |
| 3:N:1105:ILE:HD11 | 3:N:1374:GLN:CD   | 2.05                     | 0.76              |
| 3:N:1161:GLU:HG3  | 3:N:1164:ARG:HB2  | 1.68                     | 0.76              |
| 3:N:406:ASP:HB2   | 3:N:423:ASP:HA    | 1.67                     | 0.76              |
| 4:O:46:PRO:CB     | 4:O:57:ASP:HB3    | 2.15                     | 0.76              |
| 3:N:566:ILE:HG22  | 5:P:84:TYR:OH     | 1.85                     | 0.76              |
| 2:C:195:LEU:N     | 2:C:195:LEU:HD23  | 1.97                     | 0.75              |
| 2:C:599:GLU:HB3   | 2:C:615:TYR:CD2   | 2.21                     | 0.75              |
| 3:D:192:ALA:HB3   | 3:D:195:VAL:HG23  | 1.68                     | 0.75              |
| 2:M:431:HIS:CE1   | 2:M:432:ARG:HG2   | 2.21                     | 0.75              |
| 2:M:807:ARG:HB3   | 2:M:807:ARG:NH1   | 2.01                     | 0.75              |
| 3:N:329:GLU:HG2   | 3:N:330:THR:HG23  | 1.68                     | 0.75              |
| 3:N:530:VAL:HG23  | 3:N:531:ASP:H     | 1.49                     | 0.75              |
| 3:N:57:GLU:HG3    | 3:N:64:LYS:HG2    | 1.68                     | 0.75              |
| 3:N:793:THR:O     | 3:N:905:PRO:HA    | 1.87                     | 0.75              |
| 2:C:396:ASP:O     | 2:C:403:SER:HA    | 1.86                     | 0.75              |
| 2:C:607:ASP:HB3   | 2:C:610:ARG:HH12  | 1.51                     | 0.75              |
| 3:D:206:ARG:NH2   | 3:D:394:LEU:HD13  | 2.01                     | 0.75              |
| 3:D:438:ASP:HB3   | 3:D:443:VAL:O     | 1.85                     | 0.75              |
| 4:E:46:PRO:CB     | 4:E:57:ASP:HB3    | 2.15                     | 0.75              |
| 2:M:443:THR:OG1   | 2:M:444:PRO:HD2   | 1.86                     | 0.75              |
| 2:M:691:SER:HB2   | 2:M:858:MET:SD    | 2.26                     | 0.75              |
| 3:N:1208:ASP:O    | 3:N:1209:LEU:HB2  | 1.87                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:318:ARG:HB2   | 3:N:338:GLU:OE2   | 1.86                     | 0.75              |
| 3:N:400:VAL:HG23  | 3:N:443:VAL:CG1   | 2.16                     | 0.75              |
| 3:N:711:LEU:HD22  | 3:N:778:LEU:HD23  | 1.68                     | 0.75              |
| 4:O:40:LEU:HD12   | 4:O:41:GLU:N      | 2.00                     | 0.75              |
| 1:B:5:LYS:C       | 1:B:7:LYS:H       | 1.89                     | 0.75              |
| 3:D:567:ILE:HG22  | 3:D:571:LYS:HE3   | 1.68                     | 0.75              |
| 3:D:675:ARG:O     | 3:D:678:GLU:HG2   | 1.85                     | 0.75              |
| 1:K:1:MET:H1      | 1:K:6:LEU:HD13    | 1.49                     | 0.75              |
| 3:N:1117:TYR:C    | 3:N:1193:THR:HG21 | 2.07                     | 0.75              |
| 3:N:122:GLU:O     | 3:N:126:VAL:HB    | 1.87                     | 0.75              |
| 3:N:244:GLU:HG2   | 3:N:245:LEU:H     | 1.50                     | 0.75              |
| 5:P:416:ARG:NH1   | 5:P:419:ARG:HD3   | 2.00                     | 0.75              |
| 1:B:76:VAL:HA     | 1:B:79:ILE:CD1    | 2.15                     | 0.75              |
| 2:C:189:ARG:NH2   | 2:C:242:LEU:HA    | 2.02                     | 0.75              |
| 2:C:762:LYS:HG2   | 2:C:763:GLY:N     | 1.99                     | 0.75              |
| 3:D:1404:ASN:HA   | 3:D:1408:ILE:HB   | 1.67                     | 0.75              |
| 3:D:808:THR:H     | 3:D:809:PRO:CD    | 2.00                     | 0.75              |
| 1:K:186:LEU:C     | 1:K:188:GLN:H     | 1.90                     | 0.75              |
| 3:N:323:GLU:HB2   | 3:N:334:THR:HB    | 1.68                     | 0.75              |
| 3:N:417:PRO:HA    | 3:N:429:SER:O     | 1.85                     | 0.75              |
| 3:N:819:GLY:HA2   | 3:N:824:ASN:HD22  | 1.50                     | 0.75              |
| 1:A:132:LEU:HD13  | 1:A:136:GLY:O     | 1.86                     | 0.75              |
| 2:C:1014:SER:HA   | 2:C:1021:LEU:HD22 | 1.68                     | 0.75              |
| 2:C:185:LYS:HA    | 2:C:190:LYS:HB3   | 1.68                     | 0.75              |
| 2:C:266:ARG:HG3   | 2:C:266:ARG:HH11  | 1.52                     | 0.75              |
| 2:C:349:ALA:O     | 2:C:353:ARG:HG3   | 1.85                     | 0.75              |
| 3:D:610:LYS:HZ1   | 3:D:1442:ASN:H    | 1.33                     | 0.75              |
| 5:F:349:LEU:HA    | 5:F:352:GLU:OE2   | 1.86                     | 0.75              |
| 2:M:873:PRO:O     | 2:M:876:VAL:HG23  | 1.85                     | 0.75              |
| 3:N:1476:THR:HB   | 4:O:21:VAL:HG23   | 1.69                     | 0.75              |
| 3:N:769:LEU:N     | 3:N:769:LEU:HD12  | 2.01                     | 0.75              |
| 2:C:358:ARG:HD2   | 2:C:372:LEU:HA    | 1.68                     | 0.75              |
| 2:C:57:GLU:HG3    | 2:C:62:GLY:O      | 1.86                     | 0.75              |
| 3:D:1119:SER:HA   | 3:D:1186:VAL:O    | 1.87                     | 0.75              |
| 2:M:401:LEU:HD11  | 2:M:543:ASN:HB3   | 1.67                     | 0.75              |
| 2:M:834:GLN:N     | 2:M:837:ASP:OD2   | 2.20                     | 0.75              |
| 3:N:676:MET:HG3   | 3:N:677:LEU:CD2   | 2.17                     | 0.75              |
| 2:C:79:PRO:HG2    | 2:C:82:GLU:HB2    | 1.68                     | 0.75              |
| 2:C:93:PRO:N      | 2:C:117:HIS:HB3   | 2.01                     | 0.75              |
| 3:D:1281:VAL:HG23 | 3:D:1317:ASP:O    | 1.86                     | 0.75              |
| 3:D:136:ASP:CB    | 3:D:137:PRO:HD3   | 2.17                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:122:THR:HB    | 2:M:124:ASP:OD1   | 1.86                     | 0.75              |
| 2:M:300:ASP:O     | 2:M:304:LEU:HD13  | 1.86                     | 0.75              |
| 2:M:425:PHE:HE2   | 3:N:1239:ARG:HH21 | 1.34                     | 0.75              |
| 3:N:1335:LEU:CD2  | 3:N:1344:VAL:HA   | 2.16                     | 0.75              |
| 4:O:76:GLY:HA3    | 4:O:79:LEU:HD21   | 1.68                     | 0.75              |
| 2:C:91:GLN:HB2    | 2:C:118:ILE:O     | 1.87                     | 0.75              |
| 2:C:15:LEU:CD1    | 2:C:15:LEU:H      | 1.95                     | 0.75              |
| 2:C:325:ILE:HD12  | 2:C:325:ILE:N     | 2.01                     | 0.75              |
| 3:D:358:GLY:HA2   | 3:D:385:VAL:HB    | 1.67                     | 0.75              |
| 1:K:195:LEU:HD12  | 1:K:196:THR:H     | 1.50                     | 0.75              |
| 1:L:208:LEU:HG    | 1:L:209:GLU:N     | 1.99                     | 0.75              |
| 2:M:101:ILE:HG22  | 2:M:102:HIS:H     | 1.52                     | 0.75              |
| 2:M:676:ILE:HG23  | 2:M:988:VAL:HG13  | 1.69                     | 0.75              |
| 2:M:939:ARG:HD2   | 2:M:982:PRO:HD3   | 1.69                     | 0.75              |
| 3:N:1335:LEU:HD23 | 3:N:1344:VAL:HA   | 1.68                     | 0.75              |
| 3:N:284:LEU:HD13  | 3:N:288:MET:HG3   | 1.67                     | 0.75              |
| 3:N:365:ASP:O     | 3:N:379:ALA:HB2   | 1.87                     | 0.75              |
| 3:N:808:THR:H     | 3:N:809:PRO:HD2   | 1.50                     | 0.75              |
| 2:C:431:HIS:CE1   | 2:C:432:ARG:HG2   | 2.22                     | 0.75              |
| 3:D:1001:GLU:HA   | 3:D:1001:GLU:OE2  | 1.87                     | 0.75              |
| 3:D:1496:GLU:OE2  | 3:D:1500:LYS:HB2  | 1.87                     | 0.75              |
| 2:M:737:LEU:HD11  | 2:M:741:GLY:O     | 1.86                     | 0.75              |
| 3:N:1424:VAL:HG23 | 3:N:1425:THR:H    | 1.51                     | 0.75              |
| 1:A:138:LEU:HD21  | 1:A:140:MET:HE3   | 1.68                     | 0.74              |
| 2:C:709:GLU:HG2   | 2:C:824:ARG:HG2   | 1.66                     | 0.74              |
| 3:D:112:ILE:O     | 3:D:115:LEU:HB3   | 1.87                     | 0.74              |
| 3:D:1339:LYS:HB3  | 3:D:1343:ALA:HB2  | 1.69                     | 0.74              |
| 3:D:548:ILE:HG22  | 3:D:552:ASN:ND2   | 2.00                     | 0.74              |
| 3:D:567:ILE:HG21  | 5:F:140:ARG:HH12  | 1.52                     | 0.74              |
| 2:C:984:GLU:OE1   | 3:D:945:SER:HA    | 1.86                     | 0.74              |
| 4:E:25:LYS:HA     | 4:E:28:GLN:NE2    | 2.02                     | 0.74              |
| 2:M:304:LEU:CB    | 2:M:305:PRO:HD3   | 2.17                     | 0.74              |
| 3:N:1085:ALA:HA   | 3:N:1088:THR:HG22 | 1.69                     | 0.74              |
| 3:N:1372:VAL:HA   | 3:N:1375:MET:HE3  | 1.68                     | 0.74              |
| 3:N:135:LEU:HD12  | 3:N:148:GLU:HB2   | 1.67                     | 0.74              |
| 1:A:178:ALA:HB2   | 2:C:864:GLY:HA3   | 1.69                     | 0.74              |
| 1:A:42:ARG:HH12   | 1:B:34:VAL:HB     | 1.52                     | 0.74              |
| 2:C:101:ILE:HA    | 2:C:106:GLY:O     | 1.87                     | 0.74              |
| 3:D:411:THR:HB    | 3:D:437:VAL:CB    | 2.16                     | 0.74              |
| 3:D:523:ASP:HA    | 3:D:526:PRO:HG3   | 1.68                     | 0.74              |
| 3:D:811:GLU:HB2   | 3:D:816:HIS:CE1   | 2.22                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:115:LYS:O     | 5:F:119:ILE:HG13  | 1.87                     | 0.74              |
| 5:F:123:ASP:O     | 5:F:126:LEU:HB3   | 1.87                     | 0.74              |
| 1:L:101:LEU:HB3   | 1:L:140:MET:SD    | 2.27                     | 0.74              |
| 1:L:58:ILE:HG12   | 1:L:140:MET:HB2   | 1.68                     | 0.74              |
| 3:N:1095:THR:O    | 3:N:1099:VAL:HG23 | 1.87                     | 0.74              |
| 3:N:775:GLY:HA2   | 3:N:1209:LEU:O    | 1.87                     | 0.74              |
| 1:A:5:LYS:HZ1     | 1:A:192:LEU:HD22  | 1.50                     | 0.74              |
| 2:C:264:PRO:C     | 2:C:289:THR:HG21  | 2.08                     | 0.74              |
| 2:C:344:PHE:O     | 2:C:348:LEU:HB2   | 1.85                     | 0.74              |
| 3:D:119:SER:H     | 3:D:123:LEU:CD1   | 2.00                     | 0.74              |
| 5:F:386:VAL:HG23  | 5:F:387:GLY:N     | 2.03                     | 0.74              |
| 1:K:86:VAL:HG12   | 1:K:124:ASN:ND2   | 2.01                     | 0.74              |
| 3:N:1394:VAL:HG21 | 3:N:1397:LYS:HZ1  | 1.52                     | 0.74              |
| 3:N:252:ARG:HG3   | 3:N:300:LYS:C     | 2.08                     | 0.74              |
| 3:N:264:LEU:HD12  | 3:N:267:GLY:HA3   | 1.67                     | 0.74              |
| 5:P:113:ILE:HA    | 5:P:116:LEU:HD12  | 1.69                     | 0.74              |
| 2:C:300:ASP:OD2   | 2:C:302:VAL:HB    | 1.87                     | 0.74              |
| 2:C:31:GLN:O      | 2:C:35:PRO:HB2    | 1.88                     | 0.74              |
| 3:D:16:GLU:CD     | 3:D:16:GLU:H      | 1.91                     | 0.74              |
| 3:D:82:LYS:CB     | 3:D:84:ILE:HG22   | 2.18                     | 0.74              |
| 5:F:155:THR:HA    | 5:F:158:GLU:OE2   | 1.87                     | 0.74              |
| 2:M:194:VAL:HA    | 2:M:197:LEU:CD1   | 2.16                     | 0.74              |
| 2:M:626:ARG:HG3   | 2:M:629:TYR:HD1   | 1.52                     | 0.74              |
| 3:N:1098:LEU:CD1  | 3:N:1098:LEU:H    | 2.00                     | 0.74              |
| 3:D:700:VAL:O     | 3:D:715:ALA:HA    | 1.87                     | 0.74              |
| 5:F:321:ILE:HG13  | 5:F:332:PHE:CE1   | 2.22                     | 0.74              |
| 1:L:100:LEU:HD12  | 1:L:140:MET:O     | 1.88                     | 0.74              |
| 2:M:199:VAL:HG21  | 2:M:238:LEU:HD11  | 1.70                     | 0.74              |
| 3:N:1381:VAL:HG12 | 3:N:1391:GLU:O    | 1.87                     | 0.74              |
| 1:A:91:ASN:HD21   | 1:A:93:SER:HB2    | 1.53                     | 0.74              |
| 1:B:68:ILE:HG13   | 1:B:71:VAL:O      | 1.87                     | 0.74              |
| 2:C:353:ARG:HG2   | 2:C:353:ARG:HH11  | 1.52                     | 0.74              |
| 3:D:119:SER:HB3   | 3:D:123:LEU:N     | 1.98                     | 0.74              |
| 1:L:55:SER:HB2    | 1:L:165:ILE:O     | 1.88                     | 0.74              |
| 2:M:95:TYR:CD2    | 2:M:114:PHE:HB3   | 2.23                     | 0.74              |
| 2:M:163:ILE:O     | 2:M:266:ARG:HG3   | 1.87                     | 0.74              |
| 2:M:325:ILE:CD1   | 2:M:325:ILE:H     | 2.00                     | 0.74              |
| 2:M:439:CYS:HB2   | 2:M:541:SER:HB3   | 1.69                     | 0.74              |
| 3:N:1201:CYS:SG   | 3:N:1203:LYS:HB2  | 2.28                     | 0.74              |
| 3:N:119:SER:H     | 3:N:123:LEU:CB    | 2.01                     | 0.74              |
| 3:N:812:ALA:HA    | 3:N:816:HIS:HB2   | 1.69                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:81:VAL:HG23   | 5:P:82:ARG:H      | 1.52                     | 0.74              |
| 3:D:119:SER:CB    | 3:D:123:LEU:HG    | 2.18                     | 0.74              |
| 3:D:1394:VAL:HB   | 3:D:1397:LYS:CE   | 2.16                     | 0.74              |
| 3:D:241:ILE:HG13  | 3:D:312:ARG:NH1   | 2.02                     | 0.74              |
| 5:F:157:GLU:HA    | 5:F:160:ASP:OD2   | 1.88                     | 0.74              |
| 3:D:534:ARG:NE    | 5:F:314:PRO:HA    | 2.02                     | 0.74              |
| 2:M:1055:LEU:HD11 | 2:M:1079:PRO:HG3  | 1.70                     | 0.74              |
| 2:M:575:GLN:HG3   | 2:M:670:GLN:HG2   | 1.69                     | 0.74              |
| 3:N:1290:LEU:HD23 | 3:N:1307:LYS:HA   | 1.68                     | 0.74              |
| 3:N:192:ALA:HB3   | 3:N:195:VAL:CG2   | 2.17                     | 0.74              |
| 3:N:252:ARG:NH2   | 3:N:300:LYS:HG2   | 2.03                     | 0.74              |
| 3:N:432:TYR:O     | 3:N:448:GLU:HA    | 1.86                     | 0.74              |
| 3:N:890:VAL:HG23  | 3:N:892:ASP:H     | 1.52                     | 0.74              |
| 2:C:115:LEU:H     | 2:C:115:LEU:HD23  | 1.53                     | 0.74              |
| 2:C:325:ILE:H     | 2:C:325:ILE:CD1   | 2.01                     | 0.74              |
| 2:C:678:PRO:O     | 3:D:943:THR:HA    | 1.87                     | 0.74              |
| 3:D:1269:LYS:HE2  | 3:D:1270:ALA:H    | 1.53                     | 0.74              |
| 3:D:65:ARG:HG3    | 3:D:67:ARG:HG2    | 1.68                     | 0.74              |
| 3:D:864:VAL:HG12  | 3:D:865:THR:N     | 2.01                     | 0.74              |
| 4:E:7:ASP:HA      | 4:E:10:PHE:HD1    | 1.51                     | 0.74              |
| 2:M:764:GLU:O     | 2:M:766:GLU:HG3   | 1.87                     | 0.74              |
| 3:N:1080:GLY:O    | 3:N:1084:THR:HG22 | 1.88                     | 0.74              |
| 3:N:371:ILE:HD13  | 5:P:232:ARG:HD3   | 1.70                     | 0.74              |
| 2:C:232:GLU:HA    | 2:C:235:LEU:HD13  | 1.69                     | 0.74              |
| 2:C:278:GLU:OE2   | 2:C:284:ARG:HG2   | 1.87                     | 0.74              |
| 3:D:1029:ARG:NH1  | 3:D:1029:ARG:HG3  | 2.01                     | 0.74              |
| 3:D:610:LYS:NZ    | 3:D:1441:GLN:HG3  | 2.02                     | 0.74              |
| 2:C:889:HIS:HE1   | 3:D:951:ILE:H     | 1.36                     | 0.74              |
| 5:F:192:LEU:O     | 5:F:195:VAL:HB    | 1.88                     | 0.74              |
| 5:P:271:LEU:HD11  | 5:P:307:THR:HG21  | 1.70                     | 0.74              |
| 2:C:712:ALA:O     | 2:C:820:ARG:HG3   | 1.87                     | 0.74              |
| 2:C:918:LEU:HD12  | 2:C:968:LEU:HA    | 1.70                     | 0.74              |
| 3:D:119:SER:H     | 3:D:123:LEU:CG    | 2.00                     | 0.74              |
| 3:D:519:VAL:HA    | 3:D:544:TYR:OH    | 1.87                     | 0.74              |
| 5:F:386:VAL:HG23  | 5:F:387:GLY:H     | 1.53                     | 0.74              |
| 2:M:628:PHE:HD1   | 2:M:628:PHE:N     | 1.85                     | 0.74              |
| 3:N:1267:ARG:NH2  | 3:N:1271:LYS:HZ1  | 1.82                     | 0.73              |
| 3:N:133:ILE:CD1   | 3:N:456:MET:HE1   | 2.19                     | 0.73              |
| 2:C:774:LEU:HA    | 2:C:777:ILE:HD12  | 1.70                     | 0.73              |
| 2:C:674:VAL:HG21  | 2:C:871:LEU:HD12  | 1.70                     | 0.73              |
| 3:D:1066:THR:HB   | 3:D:1069:GLU:H    | 1.51                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1311:LEU:HD21 | 3:D:1313:VAL:O    | 1.86                     | 0.73              |
| 3:D:191:LEU:HD23  | 3:D:195:VAL:CG1   | 2.18                     | 0.73              |
| 1:L:18:ARG:HH12   | 1:L:88:ARG:NH2    | 1.86                     | 0.73              |
| 2:M:276:LYS:HB3   | 2:M:280:LYS:NZ    | 2.03                     | 0.73              |
| 3:N:1406:ARG:HB3  | 3:N:1412:LYS:HE2  | 1.70                     | 0.73              |
| 3:N:1464:GLU:HG2  | 3:N:1465:ASN:H    | 1.51                     | 0.73              |
| 3:N:810:GLU:O     | 3:N:813:LEU:HG    | 1.87                     | 0.73              |
| 5:P:392:VAL:HG11  | 5:P:396:ARG:HD3   | 1.69                     | 0.73              |
| 2:C:913:GLU:O     | 2:C:916:GLU:HB3   | 1.89                     | 0.73              |
| 3:D:249:TYR:HE1   | 3:D:330:THR:HG21  | 1.53                     | 0.73              |
| 4:E:31:LEU:HD21   | 4:E:60:ALA:HB2    | 1.69                     | 0.73              |
| 1:K:64:GLU:HG3    | 1:K:76:VAL:HG22   | 1.70                     | 0.73              |
| 2:C:1005:MET:HG2  | 3:D:629:SER:HB2   | 1.71                     | 0.73              |
| 2:M:673:LEU:HD21  | 2:M:895:TYR:CE1   | 2.23                     | 0.73              |
| 3:N:990:ASP:HA    | 3:N:993:LEU:HD12  | 1.70                     | 0.73              |
| 2:C:1037:VAL:O    | 2:C:1041:GLU:HG3  | 1.88                     | 0.73              |
| 2:C:91:GLN:HB2    | 2:C:118:ILE:C     | 2.07                     | 0.73              |
| 3:D:227:LEU:HD11  | 3:D:327:GLU:H     | 1.51                     | 0.73              |
| 2:M:456:ALA:HB3   | 2:M:459:ALA:HB2   | 1.70                     | 0.73              |
| 3:N:701:LEU:HB2   | 3:N:748:HIS:HB2   | 1.68                     | 0.73              |
| 3:N:853:VAL:HG13  | 3:N:858:VAL:O     | 1.88                     | 0.73              |
| 1:B:112:ARG:HB3   | 1:B:112:ARG:HH11  | 1.54                     | 0.73              |
| 1:B:86:VAL:HG12   | 1:B:124:ASN:ND2   | 2.04                     | 0.73              |
| 1:B:153:ALA:HA    | 1:B:156:HIS:HE1   | 1.51                     | 0.73              |
| 2:C:425:PHE:HZ    | 3:D:1239:ARG:HH21 | 1.35                     | 0.73              |
| 2:C:55:GLU:HG2    | 2:C:57:GLU:H      | 1.53                     | 0.73              |
| 3:D:269:PHE:HD1   | 3:D:283:PHE:HB2   | 1.53                     | 0.73              |
| 2:M:267:TYR:HB2   | 2:M:272:ALA:CB    | 2.18                     | 0.73              |
| 2:M:836:GLY:H     | 2:M:849:VAL:HB    | 1.53                     | 0.73              |
| 3:N:478:LEU:O     | 3:N:481:MET:HB3   | 1.89                     | 0.73              |
| 3:N:551:ASN:O     | 3:N:554:LEU:HB3   | 1.88                     | 0.73              |
| 3:N:86:ARG:HB3    | 3:N:523:ASP:OD2   | 1.89                     | 0.73              |
| 2:C:261:ILE:O     | 2:C:264:PRO:HD2   | 1.88                     | 0.73              |
| 2:C:439:CYS:HB2   | 2:C:541:SER:HB2   | 1.69                     | 0.73              |
| 3:D:490:ALA:O     | 3:D:494:LYS:HG2   | 1.88                     | 0.73              |
| 3:D:806:PHE:H     | 3:D:809:PRO:HG2   | 1.53                     | 0.73              |
| 5:F:245:GLN:HA    | 5:F:245:GLN:HE21  | 1.54                     | 0.73              |
| 2:M:15:LEU:HD13   | 2:M:586:ARG:HH11  | 1.53                     | 0.73              |
| 2:M:136:ILE:HD13  | 2:M:392:SER:HA    | 1.71                     | 0.73              |
| 2:M:479:VAL:HG23  | 2:M:506:ASN:O     | 1.87                     | 0.73              |
| 2:M:861:LEU:HB3   | 2:M:862:PRO:HD2   | 1.70                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:119:SER:N     | 3:N:123:LEU:HG   | 2.02                     | 0.73              |
| 3:N:260:GLU:HB2   | 3:N:271:VAL:HB   | 1.71                     | 0.73              |
| 3:N:266:GLU:HB3   | 3:N:286:VAL:HG23 | 1.71                     | 0.73              |
| 3:N:462:GLN:HG3   | 3:N:513:ILE:HG21 | 1.68                     | 0.73              |
| 3:N:618:LEU:HD22  | 5:P:326:ASP:HB2  | 1.70                     | 0.73              |
| 5:P:235:PHE:O     | 5:P:238:TYR:HB3  | 1.88                     | 0.73              |
| 2:C:334:ARG:HH11  | 2:C:418:LEU:CD1  | 2.01                     | 0.73              |
| 3:D:285:PRO:HB2   | 3:D:312:ARG:O    | 1.88                     | 0.73              |
| 3:D:48:ARG:HA     | 3:D:78:VAL:HG22  | 1.69                     | 0.73              |
| 5:F:159:ILE:O     | 5:F:162:LYS:HB2  | 1.88                     | 0.73              |
| 2:M:1086:ARG:HB3  | 2:M:1112:PHE:HE2 | 1.52                     | 0.73              |
| 3:N:139:GLY:C     | 3:N:147:VAL:HB   | 2.08                     | 0.73              |
| 3:N:399:ARG:HB3   | 3:N:401:TYR:HE1  | 1.51                     | 0.73              |
| 5:P:416:ARG:HD2   | 5:P:419:ARG:HG2  | 1.71                     | 0.73              |
| 1:A:206:THR:HG22  | 1:A:208:LEU:HB3  | 1.71                     | 0.73              |
| 3:D:1208:ASP:O    | 3:D:1209:LEU:HB2 | 1.89                     | 0.73              |
| 3:D:28:LYS:HG2    | 3:D:42:ASP:HB3   | 1.71                     | 0.73              |
| 3:D:806:PHE:HA    | 3:D:809:PRO:CD   | 2.18                     | 0.73              |
| 5:F:383:LEU:HD11  | 5:F:394:ARG:NH1  | 2.04                     | 0.73              |
| 2:M:626:ARG:HG3   | 2:M:629:TYR:CD1  | 2.24                     | 0.73              |
| 2:M:986:PRO:O     | 2:M:987:ILE:HD13 | 1.88                     | 0.73              |
| 3:N:1495:ILE:HG23 | 3:N:1496:GLU:N   | 2.03                     | 0.73              |
| 3:N:284:LEU:HD22  | 3:N:288:MET:HG2  | 1.71                     | 0.73              |
| 5:P:181:GLU:OE2   | 5:P:184:ARG:HD3  | 1.89                     | 0.73              |
| 5:P:383:LEU:CD2   | 5:P:394:ARG:HD3  | 2.19                     | 0.73              |
| 1:B:138:LEU:HD12  | 1:B:139:ASN:N    | 2.04                     | 0.73              |
| 2:C:1008:ARG:NH1  | 3:D:624:ASP:OD1  | 2.22                     | 0.73              |
| 2:C:93:PRO:CA     | 2:C:117:HIS:HB3  | 2.19                     | 0.73              |
| 2:C:987:ILE:HA    | 3:D:948:THR:HG21 | 1.70                     | 0.73              |
| 3:D:983:LEU:HD22  | 3:D:987:GLU:HB3  | 1.71                     | 0.73              |
| 4:E:40:LEU:HD12   | 4:E:41:GLU:N     | 2.01                     | 0.73              |
| 2:M:21:ILE:HD12   | 2:M:21:ILE:N     | 2.02                     | 0.73              |
| 2:M:234:ALA:O     | 2:M:238:LEU:HG   | 1.89                     | 0.73              |
| 2:M:413:LEU:CA    | 2:M:419:THR:HG21 | 2.19                     | 0.73              |
| 3:N:182:GLY:HA2   | 3:N:203:ALA:HB3  | 1.71                     | 0.73              |
| 3:N:301:GLY:C     | 3:N:303:PRO:HD2  | 2.09                     | 0.73              |
| 3:N:984:THR:HG22  | 3:N:987:GLU:CG   | 2.18                     | 0.73              |
| 5:P:111:GLU:HA    | 5:P:114:LYS:CD   | 2.18                     | 0.73              |
| 5:P:185:GLN:HA    | 5:P:188:ILE:HD12 | 1.70                     | 0.73              |
| 1:A:13:VAL:O      | 1:B:231:ALA:HB3  | 1.89                     | 0.72              |
| 2:C:176:VAL:HG12  | 2:C:183:SER:H    | 1.53                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:199:VAL:HG21 | 2:C:238:LEU:HD12  | 1.71                     | 0.72              |
| 3:D:283:PHE:O    | 3:D:284:LEU:HD23  | 1.89                     | 0.72              |
| 5:F:142:ARG:HD2  | 5:F:145:PRO:HA    | 1.71                     | 0.72              |
| 1:L:80:LEU:HB3   | 3:N:844:ALA:HB2   | 1.69                     | 0.72              |
| 2:M:293:PHE:HD1  | 2:M:294:GLU:HG3   | 1.52                     | 0.72              |
| 3:N:1085:ALA:HA  | 3:N:1088:THR:CG2  | 2.19                     | 0.72              |
| 3:N:121:THR:HG23 | 3:N:122:GLU:N     | 2.01                     | 0.72              |
| 5:P:355:GLU:O    | 5:P:358:LEU:HB3   | 1.88                     | 0.72              |
| 5:P:422:LEU:N    | 5:P:422:LEU:HD23  | 2.04                     | 0.72              |
| 1:A:1:MET:H1     | 1:A:6:LEU:HB2     | 1.54                     | 0.72              |
| 3:D:1041:LEU:HG  | 3:D:1043:GLY:N    | 2.03                     | 0.72              |
| 3:D:1238:MET:CE  | 3:D:1239:ARG:HB3  | 2.19                     | 0.72              |
| 5:F:267:THR:O    | 5:F:270:LYS:HB3   | 1.89                     | 0.72              |
| 2:M:289:THR:C    | 2:M:290:LEU:HD23  | 2.09                     | 0.72              |
| 2:M:606:VAL:HG12 | 2:M:611:ILE:HG23  | 1.70                     | 0.72              |
| 2:M:896:PHE:C    | 2:M:898:GLY:H     | 1.89                     | 0.72              |
| 3:N:1380:GLU:HG2 | 3:N:1381:VAL:N    | 2.04                     | 0.72              |
| 3:N:500:ARG:O    | 3:N:504:ASP:HB2   | 1.88                     | 0.72              |
| 3:N:410:SER:HB2  | 5:P:178:ARG:HG3   | 1.71                     | 0.72              |
| 5:P:282:LEU:HG   | 5:P:284:ARG:HG3   | 1.71                     | 0.72              |
| 2:C:180:GLY:HA2  | 2:C:223:ASP:OD2   | 1.89                     | 0.72              |
| 2:C:93:PRO:HG3   | 2:C:117:HIS:CD2   | 2.23                     | 0.72              |
| 3:D:108:VAL:HA   | 3:D:109:PRO:C     | 2.07                     | 0.72              |
| 3:D:100:ALA:HB3  | 3:D:128:TYR:CE2   | 2.23                     | 0.72              |
| 3:D:499:VAL:O    | 3:D:503:LEU:N     | 2.22                     | 0.72              |
| 3:D:530:VAL:CG2  | 3:D:531:ASP:H     | 1.94                     | 0.72              |
| 2:C:1104:GLU:HA  | 3:D:7:LYS:HZ2     | 1.50                     | 0.72              |
| 2:M:281:LEU:HB3  | 2:M:305:PRO:HB3   | 1.71                     | 0.72              |
| 3:N:241:ILE:HG12 | 3:N:312:ARG:HG3   | 1.70                     | 0.72              |
| 3:N:644:LEU:HD12 | 3:N:645:PRO:HD2   | 1.71                     | 0.72              |
| 3:N:806:PHE:CD1  | 3:N:809:PRO:HB2   | 2.24                     | 0.72              |
| 2:C:112:GLU:O    | 2:C:113:VAL:HG13  | 1.89                     | 0.72              |
| 3:D:351:MET:HG3  | 3:D:370:ALA:HB2   | 1.71                     | 0.72              |
| 3:D:972:LEU:CD2  | 3:D:972:LEU:H     | 2.02                     | 0.72              |
| 1:K:118:ALA:O    | 1:K:120:VAL:HG23  | 1.88                     | 0.72              |
| 2:M:1067:TYR:O   | 2:M:1071:ILE:HG12 | 1.89                     | 0.72              |
| 2:M:628:PHE:CD1  | 2:M:628:PHE:N     | 2.57                     | 0.72              |
| 3:N:1197:ARG:HG2 | 3:N:1198:TYR:CE2  | 2.25                     | 0.72              |
| 3:N:148:GLU:CB   | 3:N:151:GLN:HB2   | 2.18                     | 0.72              |
| 3:N:361:VAL:CG1  | 3:N:365:ASP:HB3   | 2.14                     | 0.72              |
| 3:N:550:ARG:NH1  | 3:N:573:MET:HB3   | 2.04                     | 0.72              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:97:VAL:HG12  | 1:B:98:THR:N      | 2.04                     | 0.72              |
| 2:C:334:ARG:HB2  | 2:C:339:LEU:HD21  | 1.72                     | 0.72              |
| 5:F:169:GLU:O    | 5:F:172:ARG:HG2   | 1.90                     | 0.72              |
| 5:F:181:GLU:O    | 5:F:184:ARG:HB3   | 1.90                     | 0.72              |
| 5:F:382:THR:O    | 5:F:386:VAL:HG13  | 1.89                     | 0.72              |
| 2:M:1100:GLN:HG3 | 2:M:1102:LEU:CD2  | 2.19                     | 0.72              |
| 2:M:599:GLU:HB3  | 2:M:615:TYR:CD2   | 2.24                     | 0.72              |
| 3:N:1130:ARG:NH2 | 3:N:1323:GLN:HE22 | 1.87                     | 0.72              |
| 1:B:74:ASP:O     | 1:B:77:GLU:HB3    | 1.89                     | 0.72              |
| 3:D:192:ALA:HB3  | 3:D:195:VAL:CG2   | 2.19                     | 0.72              |
| 3:D:245:LEU:H    | 3:D:309:GLY:N     | 1.87                     | 0.72              |
| 3:D:248:PRO:HB3  | 3:D:308:LYS:HZ1   | 1.53                     | 0.72              |
| 4:E:6:ILE:HG23   | 4:E:7:ASP:N       | 2.04                     | 0.72              |
| 2:M:101:ILE:HG12 | 2:M:107:LEU:HA    | 1.70                     | 0.72              |
| 3:N:804:LEU:O    | 3:N:809:PRO:HG2   | 1.90                     | 0.72              |
| 5:P:280:GLN:HG3  | 5:P:281:GLU:N     | 2.05                     | 0.72              |
| 1:A:152:PRO:HB2  | 1:A:154:GLU:OE1   | 1.89                     | 0.72              |
| 1:B:74:ASP:HB3   | 1:B:77:GLU:HB2    | 1.70                     | 0.72              |
| 3:D:1172:HIS:O   | 3:D:1175:ILE:HB   | 1.88                     | 0.72              |
| 3:D:1083:ASP:HB2 | 3:D:1239:ARG:HH22 | 1.52                     | 0.72              |
| 3:D:355:VAL:CG2  | 3:D:367:ILE:HG23  | 2.20                     | 0.72              |
| 5:F:402:ASN:HB3  | 5:F:406:ARG:CZ    | 2.19                     | 0.72              |
| 1:K:182:GLU:HG3  | 1:K:194:LYS:HD3   | 1.70                     | 0.72              |
| 2:M:1007:ALA:CB  | 3:N:648:MET:HG3   | 2.18                     | 0.72              |
| 2:M:512:ARG:HG3  | 2:M:523:ILE:HD11  | 1.71                     | 0.72              |
| 2:M:676:ILE:HG12 | 2:M:873:PRO:HG3   | 1.72                     | 0.72              |
| 2:M:881:ASN:N    | 2:M:881:ASN:HD22  | 1.85                     | 0.72              |
| 3:N:274:ARG:HE   | 3:N:279:VAL:HG11  | 1.55                     | 0.72              |
| 2:C:1063:ARG:O   | 2:C:1066:ALA:HB3  | 1.89                     | 0.72              |
| 2:C:631:SER:HA   | 2:C:637:LEU:HD11  | 1.71                     | 0.72              |
| 2:C:841:ASN:HD21 | 2:C:845:ASN:HB3   | 1.54                     | 0.72              |
| 3:D:30:GLU:HB3   | 3:D:40:GLU:CG     | 2.20                     | 0.72              |
| 3:D:368:VAL:H    | 3:D:377:VAL:HB    | 1.55                     | 0.72              |
| 3:D:358:GLY:HA2  | 3:D:385:VAL:O     | 1.89                     | 0.72              |
| 3:D:441:ARG:O    | 3:D:441:ARG:HG2   | 1.90                     | 0.72              |
| 3:D:462:GLN:HG3  | 3:D:513:ILE:HG21  | 1.70                     | 0.72              |
| 3:D:803:GLY:C    | 3:D:805:GLU:H     | 1.92                     | 0.72              |
| 5:F:208:SER:O    | 5:F:212:LEU:HG    | 1.90                     | 0.72              |
| 5:F:351:SER:HA   | 5:F:354:LEU:HD12  | 1.72                     | 0.72              |
| 2:M:224:GLU:HB3  | 2:M:227:PHE:HB2   | 1.72                     | 0.72              |
| 3:N:1001:GLU:OE2 | 3:N:1001:GLU:HA   | 1.88                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:1114:THR:HB  | 3:N:1195:GLN:CD   | 2.10                     | 0.72              |
| 3:N:525:ARG:HG2  | 3:N:525:ARG:HH11  | 1.54                     | 0.72              |
| 5:P:213:ILE:HG22 | 5:P:217:ASN:HD21  | 1.55                     | 0.72              |
| 2:C:182:VAL:HG22 | 2:C:220:GLY:O     | 1.89                     | 0.72              |
| 3:D:1479:ASP:HA  | 3:D:1482:ARG:HE   | 1.55                     | 0.72              |
| 3:D:1500:LYS:C   | 3:D:1502:ALA:H    | 1.92                     | 0.72              |
| 5:F:265:VAL:HG12 | 5:F:269:ASN:HD21  | 1.52                     | 0.72              |
| 1:K:176:ARG:CZ   | 2:M:865:THR:HG22  | 2.20                     | 0.72              |
| 3:N:297:ILE:HG23 | 3:N:298:VAL:N     | 2.05                     | 0.72              |
| 1:A:9:PRO:HG3    | 1:A:27:PRO:O      | 1.89                     | 0.72              |
| 2:C:204:GLN:O    | 2:C:209:ARG:HD3   | 1.89                     | 0.72              |
| 3:D:154:THR:HG22 | 3:D:157:GLU:CD    | 2.10                     | 0.72              |
| 3:D:204:LEU:O    | 3:D:393:ILE:HG23  | 1.90                     | 0.72              |
| 3:D:927:THR:O    | 3:D:930:LEU:HB3   | 1.90                     | 0.72              |
| 5:F:274:THR:O    | 5:F:278:LEU:HG    | 1.90                     | 0.72              |
| 1:K:5:LYS:HE3    | 1:K:29:GLU:OE1    | 1.90                     | 0.72              |
| 2:M:309:TYR:CE2  | 2:M:321:GLU:HG3   | 2.25                     | 0.72              |
| 3:N:1074:SER:O   | 3:N:1077:ALA:HB3  | 1.90                     | 0.72              |
| 3:N:367:ILE:HB   | 3:N:377:VAL:HG12  | 1.71                     | 0.72              |
| 3:N:89:ARG:HH11  | 3:N:89:ARG:HG2    | 1.55                     | 0.72              |
| 1:B:112:ARG:NH1  | 1:B:125:PRO:HB2   | 2.05                     | 0.71              |
| 2:C:654:LEU:O    | 2:C:655:LEU:HD23  | 1.89                     | 0.71              |
| 3:D:140:ALA:H    | 3:D:450:TYR:HE2   | 1.33                     | 0.71              |
| 3:D:1428:ALA:O   | 3:D:1431:THR:HG23 | 1.90                     | 0.71              |
| 3:D:187:LYS:HA   | 3:D:198:ARG:O     | 1.89                     | 0.71              |
| 3:D:704:ARG:HB2  | 3:D:745:MET:SD    | 2.29                     | 0.71              |
| 3:D:916:TYR:CE2  | 3:D:920:LEU:HD11  | 2.25                     | 0.71              |
| 2:C:679:PHE:HA   | 3:D:943:THR:HG23  | 1.72                     | 0.71              |
| 1:K:49:PRO:HA    | 1:K:148:VAL:HG12  | 1.72                     | 0.71              |
| 3:N:563:PRO:O    | 3:N:566:ILE:HG12  | 1.90                     | 0.71              |
| 3:N:828:LYS:N    | 3:N:828:LYS:HD3   | 2.05                     | 0.71              |
| 3:D:1499:ARG:HG3 | 3:D:1499:ARG:HH11 | 1.54                     | 0.71              |
| 3:D:181:ASP:C    | 3:D:183:GLU:H     | 1.93                     | 0.71              |
| 3:D:827:ILE:HG23 | 3:D:837:GLY:HA3   | 1.72                     | 0.71              |
| 1:K:12:THR:HG22  | 1:L:229:GLN:CG    | 2.20                     | 0.71              |
| 1:K:189:ARG:HB3  | 1:K:192:LEU:HD21  | 1.72                     | 0.71              |
| 2:M:398:THR:CA   | 2:M:633:GLN:HG3   | 2.21                     | 0.71              |
| 2:M:810:ASP:N    | 2:M:811:PRO:HD2   | 2.05                     | 0.71              |
| 3:N:1159:ARG:C   | 3:N:1160:LEU:HD23 | 2.11                     | 0.71              |
| 3:N:128:TYR:HA   | 3:N:457:GLY:HA2   | 1.71                     | 0.71              |
| 3:N:1405:GLU:OE1 | 3:N:1406:ARG:HG3  | 1.91                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1461:GLY:O    | 3:N:1473:PRO:HG2 | 1.89                     | 0.71              |
| 3:N:149:LYS:N     | 3:N:149:LYS:HD3  | 2.05                     | 0.71              |
| 3:N:463:GLN:HB3   | 3:N:467:GLU:OE2  | 1.91                     | 0.71              |
| 2:C:44:ILE:HG23   | 2:C:344:PHE:CE1  | 2.24                     | 0.71              |
| 2:C:328:LEU:HG    | 2:C:433:THR:OG1  | 1.89                     | 0.71              |
| 2:C:987:ILE:HD11  | 3:D:946:GLY:HA2  | 1.72                     | 0.71              |
| 3:D:1066:THR:H    | 3:D:1069:GLU:HB2 | 1.55                     | 0.71              |
| 5:F:158:GLU:O     | 5:F:162:LYS:HG3  | 1.89                     | 0.71              |
| 5:F:208:SER:HB3   | 5:F:211:ASP:OD2  | 1.90                     | 0.71              |
| 1:K:5:LYS:HE3     | 1:K:29:GLU:CD    | 2.11                     | 0.71              |
| 3:N:224:ARG:HB3   | 3:N:249:TYR:HH   | 1.55                     | 0.71              |
| 3:N:992:ILE:O     | 3:N:995:LEU:HB3  | 1.90                     | 0.71              |
| 4:O:41:GLU:CB     | 4:O:42:PRO:HD2   | 2.19                     | 0.71              |
| 2:C:211:LEU:C     | 2:C:213:ALA:H    | 1.89                     | 0.71              |
| 2:C:368:THR:CB    | 2:C:369:PRO:HD3  | 2.19                     | 0.71              |
| 2:M:274:ARG:NH2   | 2:M:284:ARG:HB3  | 2.02                     | 0.71              |
| 2:M:463:GLU:N     | 2:M:463:GLU:CD   | 2.43                     | 0.71              |
| 3:N:807:ALA:HA    | 3:N:833:GLU:CG   | 2.21                     | 0.71              |
| 1:A:111:ALA:HA    | 1:A:129:ILE:HD11 | 1.72                     | 0.71              |
| 2:C:346:VAL:HG23  | 2:C:347:GLY:N    | 2.04                     | 0.71              |
| 2:C:595:LEU:O     | 2:C:654:LEU:HD12 | 1.89                     | 0.71              |
| 3:D:1217:ILE:CD1  | 3:D:1217:ILE:H   | 1.93                     | 0.71              |
| 3:D:127:LEU:HD23  | 3:D:128:TYR:CA   | 2.19                     | 0.71              |
| 3:D:85:VAL:HG21   | 3:D:89:ARG:NE    | 2.06                     | 0.71              |
| 3:D:887:ALA:HB1   | 3:D:893:GLU:HA   | 1.72                     | 0.71              |
| 5:F:358:LEU:HD21  | 5:F:370:LYS:HZ2  | 1.55                     | 0.71              |
| 2:M:976:ASP:OD2   | 2:M:978:ARG:HB2  | 1.91                     | 0.71              |
| 3:N:357:GLU:CD    | 3:N:357:GLU:H    | 1.94                     | 0.71              |
| 4:O:40:LEU:HD13   | 4:O:72:ARG:NH1   | 2.04                     | 0.71              |
| 2:C:1060:ILE:O    | 2:C:1063:ARG:HG2 | 1.91                     | 0.71              |
| 2:C:477:GLY:HA2   | 2:C:508:ILE:CD1  | 2.21                     | 0.71              |
| 2:C:760:SER:O     | 2:C:785:VAL:HA   | 1.90                     | 0.71              |
| 3:D:250:LEU:HD11  | 3:D:304:LEU:HD22 | 1.71                     | 0.71              |
| 3:N:1149:LEU:HD23 | 3:N:1161:GLU:O   | 1.90                     | 0.71              |
| 3:N:1495:ILE:HG23 | 3:N:1496:GLU:H   | 1.55                     | 0.71              |
| 3:N:274:ARG:HB3   | 3:N:279:VAL:CG2  | 2.20                     | 0.71              |
| 3:N:48:ARG:HA     | 3:N:78:VAL:HG22  | 1.70                     | 0.71              |
| 3:N:806:PHE:CA    | 3:N:809:PRO:HD2  | 2.20                     | 0.71              |
| 1:A:206:THR:CG2   | 1:A:208:LEU:HB3  | 2.20                     | 0.71              |
| 2:C:208:ALA:HB2   | 2:C:221:LEU:CD2  | 2.21                     | 0.71              |
| 2:C:672:VAL:CG2   | 2:C:868:ASP:HB2  | 2.21                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:221:ALA:O     | 3:D:334:THR:HA    | 1.91                     | 0.71              |
| 3:D:408:GLU:CD    | 3:D:422:ALA:HB2   | 2.11                     | 0.71              |
| 3:D:699:VAL:HG12  | 3:D:717:GLN:HG2   | 1.71                     | 0.71              |
| 3:D:826:PRO:HD2   | 3:D:829:VAL:HG21  | 1.71                     | 0.71              |
| 2:M:304:LEU:HB3   | 2:M:305:PRO:CD    | 2.17                     | 0.71              |
| 3:N:209:ARG:HA    | 3:N:347:VAL:HB    | 1.71                     | 0.71              |
| 3:N:272:LEU:HD12  | 3:N:280:ALA:CB    | 2.13                     | 0.71              |
| 5:P:264:MET:CE    | 5:P:264:MET:HA    | 2.19                     | 0.71              |
| 5:P:78:SER:C      | 5:P:80:PRO:HD3    | 2.11                     | 0.71              |
| 5:P:90:GLN:O      | 5:P:92:PRO:HD3    | 1.90                     | 0.71              |
| 3:D:120:ALA:HA    | 3:D:124:GLU:OE2   | 1.90                     | 0.71              |
| 3:D:508:ARG:HB3   | 3:D:510:GLU:OE1   | 1.90                     | 0.71              |
| 5:F:409:LYS:HD2   | 5:F:410:TYR:N     | 2.05                     | 0.71              |
| 1:L:61:VAL:HG23   | 1:L:163:ASN:HB3   | 1.72                     | 0.71              |
| 2:M:199:VAL:HG21  | 2:M:238:LEU:CD1   | 2.20                     | 0.71              |
| 2:M:480:THR:HG22  | 2:M:482:GLU:H     | 1.56                     | 0.71              |
| 3:N:224:ARG:HB3   | 3:N:249:TYR:OH    | 1.90                     | 0.71              |
| 1:A:224:TYR:N     | 1:A:224:TYR:CD2   | 2.59                     | 0.71              |
| 1:B:87:VAL:HG12   | 1:B:122:ILE:HG12  | 1.71                     | 0.71              |
| 2:C:302:VAL:O     | 2:C:305:PRO:HD2   | 1.91                     | 0.71              |
| 2:C:305:PRO:HA    | 2:C:308:ARG:HE    | 1.53                     | 0.71              |
| 2:C:31:GLN:HA     | 2:C:35:PRO:HG2    | 1.70                     | 0.71              |
| 3:D:1152:GLU:HG2  | 3:D:1153:VAL:N    | 2.05                     | 0.71              |
| 3:D:1155:VAL:HG12 | 3:D:1156:LEU:HG   | 1.73                     | 0.71              |
| 3:D:1378:TYR:HB2  | 3:D:1422:MET:CE   | 2.20                     | 0.71              |
| 3:D:1486:VAL:HG21 | 4:E:22:VAL:HG13   | 1.73                     | 0.71              |
| 3:D:284:LEU:HB3   | 3:D:288:MET:HB3   | 1.72                     | 0.71              |
| 3:D:252:ARG:HG3   | 3:D:300:LYS:HA    | 1.73                     | 0.71              |
| 3:D:407:VAL:HG22  | 3:D:408:GLU:H     | 1.56                     | 0.71              |
| 3:D:138:LYS:HB3   | 3:D:450:TYR:OH    | 1.91                     | 0.71              |
| 2:C:1043:TYR:CE1  | 3:D:710:ARG:HB2   | 2.26                     | 0.71              |
| 5:F:214:GLN:O     | 5:F:217:ASN:HB2   | 1.91                     | 0.71              |
| 5:F:81:VAL:CG2    | 5:F:82:ARG:H      | 2.03                     | 0.71              |
| 1:L:47:SER:O      | 1:L:48:ILE:HD12   | 1.91                     | 0.71              |
| 2:M:537:LYS:HA    | 2:M:545:ASN:OD1   | 1.91                     | 0.71              |
| 3:N:1217:ILE:H    | 3:N:1217:ILE:CD1  | 1.96                     | 0.71              |
| 3:N:307:ALA:HB1   | 3:N:311:LEU:HD11  | 1.72                     | 0.71              |
| 5:P:295:MET:HG3   | 5:P:299:TRP:CE2   | 2.26                     | 0.71              |
| 1:A:49:PRO:HA     | 1:A:148:VAL:HG12  | 1.70                     | 0.71              |
| 3:D:1388:ARG:HH21 | 3:D:1390:LEU:HD23 | 1.52                     | 0.71              |
| 3:D:148:GLU:CB    | 3:D:151:GLN:HB2   | 2.20                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:358:GLY:CA   | 3:D:385:VAL:HB   | 2.21                     | 0.71              |
| 3:D:406:ASP:HB2  | 3:D:423:ASP:HA   | 1.73                     | 0.71              |
| 3:D:680:GLN:HA   | 3:D:683:ILE:CD1  | 2.21                     | 0.71              |
| 3:N:563:PRO:O    | 3:N:567:ILE:HG12 | 1.91                     | 0.71              |
| 5:P:81:VAL:HG23  | 5:P:82:ARG:N     | 2.05                     | 0.71              |
| 1:B:19:GLU:HA    | 1:B:201:THR:OG1  | 1.91                     | 0.70              |
| 3:D:540:LEU:HA   | 3:D:543:LEU:HD12 | 1.73                     | 0.70              |
| 3:D:610:LYS:HZ1  | 3:D:1441:GLN:HG3 | 1.54                     | 0.70              |
| 3:D:777:PRO:O    | 3:D:780:LYS:HD3  | 1.91                     | 0.70              |
| 5:F:101:GLU:O    | 5:F:105:LYS:HG3  | 1.90                     | 0.70              |
| 2:M:175:GLU:HB3  | 2:M:185:LYS:HE3  | 1.73                     | 0.70              |
| 2:M:889:HIS:HD1  | 2:M:970:GLY:HA3  | 1.55                     | 0.70              |
| 3:N:153:LEU:CD1  | 3:N:157:GLU:HB3  | 2.21                     | 0.70              |
| 3:N:237:LYS:CB   | 3:N:238:PRO:HD2  | 2.16                     | 0.70              |
| 3:N:591:VAL:HG12 | 3:N:599:PRO:HA   | 1.71                     | 0.70              |
| 5:P:151:LEU:HD13 | 5:P:154:LYS:HD2  | 1.72                     | 0.70              |
| 5:P:210:LEU:CA   | 5:P:213:ILE:HD12 | 2.19                     | 0.70              |
| 5:P:373:LYS:HZ2  | 5:P:373:LYS:HB3  | 1.56                     | 0.70              |
| 1:B:5:LYS:C      | 1:B:7:LYS:N      | 2.42                     | 0.70              |
| 2:C:266:ARG:HD2  | 2:C:273:GLY:N    | 2.06                     | 0.70              |
| 3:D:1153:VAL:HB  | 3:D:1160:LEU:HB2 | 1.72                     | 0.70              |
| 1:L:57:TYR:HE1   | 1:L:163:ASN:HB2  | 1.54                     | 0.70              |
| 2:M:100:LEU:HD23 | 2:M:368:THR:HG23 | 1.73                     | 0.70              |
| 3:N:119:SER:CB   | 3:N:123:LEU:HG   | 2.20                     | 0.70              |
| 3:N:135:LEU:N    | 3:N:135:LEU:HD23 | 2.07                     | 0.70              |
| 3:N:632:VAL:O    | 3:N:728:LEU:N    | 2.22                     | 0.70              |
| 5:P:175:HIS:O    | 5:P:178:ARG:HB2  | 1.91                     | 0.70              |
| 5:P:383:LEU:O    | 5:P:386:VAL:HG22 | 1.90                     | 0.70              |
| 1:A:195:LEU:HD12 | 1:A:196:THR:N    | 2.05                     | 0.70              |
| 2:C:192:PRO:O    | 2:C:195:LEU:HG   | 1.91                     | 0.70              |
| 2:C:839:LEU:HD23 | 2:C:996:LYS:HA   | 1.73                     | 0.70              |
| 3:D:1496:GLU:HA  | 3:D:1499:ARG:HB3 | 1.73                     | 0.70              |
| 3:D:800:LYS:HE3  | 3:D:826:PRO:CD   | 2.20                     | 0.70              |
| 5:F:94:LEU:HG    | 5:F:190:ALA:HB1  | 1.74                     | 0.70              |
| 1:K:9:PRO:HG2    | 1:K:28:LEU:HD21  | 1.73                     | 0.70              |
| 3:N:191:LEU:HD23 | 3:N:195:VAL:CG1  | 2.22                     | 0.70              |
| 3:N:490:ALA:O    | 3:N:494:LYS:HG2  | 1.90                     | 0.70              |
| 3:N:563:PRO:HD2  | 3:N:566:ILE:HD11 | 1.72                     | 0.70              |
| 5:P:214:GLN:CA   | 5:P:217:ASN:HD22 | 2.03                     | 0.70              |
| 2:C:37:GLU:HG2   | 2:C:71:TYR:HE2   | 1.56                     | 0.70              |
| 3:D:185:VAL:HA   | 3:D:189:GLN:NE2  | 2.06                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:807:ALA:HA    | 3:D:833:GLU:HG2  | 1.73                     | 0.70              |
| 2:M:89:THR:HA     | 2:M:128:ILE:O    | 1.91                     | 0.70              |
| 2:M:299:LYS:HE2   | 2:M:301:GLU:HG3  | 1.73                     | 0.70              |
| 2:M:643:VAL:HG23  | 2:M:647:GLN:CD   | 2.12                     | 0.70              |
| 3:N:1155:VAL:HG12 | 3:N:1156:LEU:HG  | 1.72                     | 0.70              |
| 3:N:1496:GLU:OE2  | 3:N:1500:LYS:HG3 | 1.91                     | 0.70              |
| 3:N:178:LEU:HG    | 3:N:181:ASP:HB2  | 1.71                     | 0.70              |
| 3:N:327:GLU:HG3   | 3:N:327:GLU:O    | 1.91                     | 0.70              |
| 3:N:522:PRO:HA    | 3:N:525:ARG:NH1  | 2.06                     | 0.70              |
| 3:N:82:LYS:CB     | 3:N:84:ILE:HG22  | 2.22                     | 0.70              |
| 1:B:5:LYS:HE2     | 1:B:189:ARG:NH1  | 2.05                     | 0.70              |
| 2:C:503:LEU:HG    | 2:C:504:GLU:H    | 1.57                     | 0.70              |
| 2:C:640:ARG:HD2   | 2:C:642:ARG:NH2  | 2.05                     | 0.70              |
| 2:C:892:LEU:O     | 2:C:895:TYR:HB3  | 1.91                     | 0.70              |
| 3:D:118:LEU:HD22  | 3:D:123:LEU:HB3  | 1.72                     | 0.70              |
| 3:D:864:VAL:HG12  | 3:D:865:THR:H    | 1.56                     | 0.70              |
| 2:M:50:GLU:C      | 2:M:52:PHE:H     | 1.93                     | 0.70              |
| 2:M:15:LEU:HD13   | 2:M:586:ARG:NH1  | 2.07                     | 0.70              |
| 2:M:398:THR:HA    | 2:M:633:GLN:HG3  | 1.72                     | 0.70              |
| 2:M:808:ARG:HG2   | 2:M:820:ARG:O    | 1.91                     | 0.70              |
| 3:N:1307:LYS:HE3  | 3:N:1307:LYS:H   | 1.55                     | 0.70              |
| 3:N:441:ARG:O     | 3:N:441:ARG:NE   | 2.24                     | 0.70              |
| 3:N:800:LYS:O     | 3:N:830:ALA:HB3  | 1.91                     | 0.70              |
| 5:P:260:ILE:HG13  | 5:P:261:PRO:HD2  | 1.72                     | 0.70              |
| 2:C:175:GLU:O     | 2:C:183:SER:HB2  | 1.91                     | 0.70              |
| 2:C:185:LYS:HE2   | 2:C:190:LYS:HZ2  | 1.57                     | 0.70              |
| 2:C:283:ILE:HG22  | 2:C:284:ARG:N    | 2.01                     | 0.70              |
| 2:C:904:PRO:HD2   | 2:C:908:GLY:CA   | 2.21                     | 0.70              |
| 3:D:676:MET:HG3   | 3:D:677:LEU:HD23 | 1.73                     | 0.70              |
| 4:E:88:GLU:O      | 4:E:92:ILE:HG13  | 1.91                     | 0.70              |
| 5:F:207:LEU:HB3   | 5:F:212:LEU:CD2  | 2.20                     | 0.70              |
| 5:F:306:GLU:O     | 5:F:310:ILE:HG13 | 1.92                     | 0.70              |
| 2:M:261:ILE:HG22  | 2:M:262:ALA:N    | 2.07                     | 0.70              |
| 3:N:206:ARG:HG2   | 3:N:392:SER:O    | 1.90                     | 0.70              |
| 5:P:289:GLU:H     | 5:P:289:GLU:CD   | 1.95                     | 0.70              |
| 2:C:257:VAL:HA    | 2:C:261:ILE:CD1  | 2.19                     | 0.70              |
| 2:C:626:ARG:HG3   | 2:C:626:ARG:HH11 | 1.55                     | 0.70              |
| 3:D:833:GLU:CD    | 3:D:833:GLU:H    | 1.93                     | 0.70              |
| 2:M:334:ARG:HB2   | 2:M:339:LEU:HD21 | 1.74                     | 0.70              |
| 2:M:693:GLU:HG3   | 2:M:697:ARG:NH1  | 2.07                     | 0.70              |
| 3:N:142:LEU:HD13  | 3:N:144:GLY:N    | 2.07                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:669:ASN:OD1   | 3:N:672:ALA:HB2  | 1.92                     | 0.70              |
| 3:N:966:GLU:O     | 3:N:969:ARG:HG2  | 1.92                     | 0.70              |
| 1:A:76:VAL:HG12   | 1:A:80:LEU:HD21  | 1.73                     | 0.70              |
| 2:C:910:LYS:HG2   | 2:C:913:GLU:CG   | 2.21                     | 0.70              |
| 3:D:1074:SER:O    | 3:D:1077:ALA:HB3 | 1.92                     | 0.70              |
| 3:D:264:LEU:HD22  | 3:D:316:GLN:HE21 | 1.57                     | 0.70              |
| 3:D:690:ALA:O     | 3:D:693:GLU:HB3  | 1.92                     | 0.70              |
| 5:F:288:TYR:HB3   | 5:F:301:ALA:HA   | 1.73                     | 0.70              |
| 2:M:470:PRO:HB2   | 2:M:534:VAL:HG21 | 1.73                     | 0.70              |
| 2:M:75:GLU:O      | 2:M:77:PRO:HD3   | 1.91                     | 0.70              |
| 3:N:1481:VAL:HG13 | 4:O:18:ARG:HA    | 1.73                     | 0.70              |
| 3:N:209:ARG:NH2   | 3:N:391:ALA:HA   | 2.07                     | 0.70              |
| 3:N:525:ARG:N     | 3:N:526:PRO:HD3  | 2.05                     | 0.70              |
| 3:N:820:GLU:HG3   | 3:N:836:VAL:HG11 | 1.74                     | 0.70              |
| 3:N:882:PHE:CE1   | 3:N:906:GLN:HG3  | 2.26                     | 0.70              |
| 3:N:932:ASP:O     | 3:N:935:LYS:HB3  | 1.92                     | 0.70              |
| 4:O:6:ILE:HG13    | 4:O:10:PHE:CE1   | 2.27                     | 0.70              |
| 5:P:219:GLY:CA    | 5:P:246:ALA:HB2  | 2.22                     | 0.70              |
| 5:P:234:LYS:HE2   | 5:P:236:SER:HB3  | 1.74                     | 0.70              |
| 2:C:115:LEU:CD1   | 2:C:373:VAL:HG12 | 2.21                     | 0.70              |
| 3:D:408:GLU:HG3   | 3:D:421:LEU:O    | 1.92                     | 0.70              |
| 2:C:1103:ASP:O    | 3:D:7:LYS:HD2    | 1.92                     | 0.70              |
| 5:F:234:LYS:HE2   | 5:F:236:SER:CB   | 2.21                     | 0.70              |
| 5:P:330:GLY:HA2   | 5:P:333:ILE:HD13 | 1.72                     | 0.70              |
| 2:C:151:ASP:H     | 2:C:158:TYR:CA   | 2.05                     | 0.70              |
| 2:C:266:ARG:NH1   | 2:C:266:ARG:HG3  | 2.07                     | 0.70              |
| 2:C:808:ARG:HG2   | 2:C:815:LEU:HD12 | 1.73                     | 0.70              |
| 3:D:1173:LEU:O    | 3:D:1176:LYS:HB3 | 1.92                     | 0.70              |
| 3:D:147:VAL:CG2   | 3:D:148:GLU:H    | 2.05                     | 0.70              |
| 1:K:214:ALA:HA    | 1:K:217:ILE:HD12 | 1.73                     | 0.70              |
| 3:N:245:LEU:HD23  | 3:N:309:GLY:N    | 2.05                     | 0.70              |
| 3:N:47:GLU:HB2    | 3:N:51:GLY:O     | 1.91                     | 0.70              |
| 4:O:46:PRO:HB2    | 4:O:57:ASP:HB3   | 1.74                     | 0.70              |
| 3:D:760:ARG:NH1   | 4:E:61:GLU:HB2   | 2.07                     | 0.69              |
| 3:D:761:ILE:HD12  | 4:E:20:THR:HG23  | 1.73                     | 0.69              |
| 3:D:805:GLU:HA    | 3:D:831:GLY:HA2  | 1.72                     | 0.69              |
| 5:F:189:GLU:HA    | 5:F:192:LEU:CG   | 2.20                     | 0.69              |
| 5:F:210:LEU:CA    | 5:F:213:ILE:HD12 | 2.12                     | 0.69              |
| 5:F:214:GLN:CA    | 5:F:217:ASN:HD22 | 2.04                     | 0.69              |
| 1:L:197:LEU:HD12  | 1:L:198:ARG:N    | 2.06                     | 0.69              |
| 2:M:948:GLU:HB3   | 2:M:953:VAL:HG23 | 1.74                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:325:GLU:CG    | 3:N:332:TYR:HB3   | 2.21                     | 0.69              |
| 3:N:32:ILE:HG22   | 3:N:33:ASN:O      | 1.91                     | 0.69              |
| 3:N:998:GLU:O     | 3:N:1001:GLU:HB3  | 1.91                     | 0.69              |
| 5:P:329:TYR:HD1   | 5:P:333:ILE:HD11  | 1.55                     | 0.69              |
| 2:C:861:LEU:N     | 2:C:861:LEU:HD23  | 2.07                     | 0.69              |
| 3:D:882:PHE:HA    | 3:D:885:ILE:HD12  | 1.73                     | 0.69              |
| 2:C:676:ILE:O     | 3:D:948:THR:HG22  | 1.91                     | 0.69              |
| 5:P:184:ARG:HG2   | 5:P:188:ILE:HD11  | 1.73                     | 0.69              |
| 2:C:737:LEU:HD12  | 2:C:742:VAL:C     | 2.11                     | 0.69              |
| 2:C:939:ARG:NH2   | 2:C:981:GLU:HG2   | 2.07                     | 0.69              |
| 5:F:288:TYR:HB2   | 5:F:289:GLU:OE2   | 1.91                     | 0.69              |
| 1:K:101:LEU:HD12  | 1:K:102:LYS:H     | 1.57                     | 0.69              |
| 2:M:41:ASN:ND2    | 2:M:46:ALA:HB2    | 2.07                     | 0.69              |
| 3:N:1081:GLY:O    | 3:N:1084:THR:HG23 | 1.92                     | 0.69              |
| 3:N:419:ASP:O     | 3:N:428:LYS:HE2   | 1.91                     | 0.69              |
| 5:P:322:GLY:O     | 5:P:324:GLU:HG3   | 1.91                     | 0.69              |
| 5:P:386:VAL:HG23  | 5:P:387:GLY:N     | 2.07                     | 0.69              |
| 2:C:182:VAL:HG21  | 2:C:194:VAL:HG23  | 1.75                     | 0.69              |
| 3:D:135:LEU:HD12  | 3:D:148:GLU:O     | 1.92                     | 0.69              |
| 1:B:185:ARG:NH2   | 3:D:692:GLU:HG3   | 2.08                     | 0.69              |
| 5:F:115:LYS:HA    | 5:F:118:GLU:OE2   | 1.92                     | 0.69              |
| 2:M:177:GLU:O     | 2:M:181:VAL:HB    | 1.93                     | 0.69              |
| 2:M:448:ASN:HB3   | 2:M:452:ILE:HD12  | 1.75                     | 0.69              |
| 2:M:71:TYR:HD2    | 2:M:71:TYR:H      | 1.40                     | 0.69              |
| 3:N:1381:VAL:HG11 | 3:N:1391:GLU:HB2  | 1.75                     | 0.69              |
| 3:N:860:LEU:HA    | 3:N:877:PRO:HB2   | 1.74                     | 0.69              |
| 5:P:312:GLN:OE1   | 5:P:312:GLN:HA    | 1.92                     | 0.69              |
| 1:A:11:PHE:O      | 1:B:229:GLN:HB3   | 1.92                     | 0.69              |
| 1:B:86:VAL:HG12   | 1:B:124:ASN:HD21  | 1.57                     | 0.69              |
| 3:D:1472:ILE:HD13 | 3:D:1473:PRO:CD   | 2.23                     | 0.69              |
| 3:D:212:ARG:HA    | 3:D:343:LYS:O     | 1.92                     | 0.69              |
| 3:D:322:VAL:HG23  | 3:D:335:LEU:HD11  | 1.74                     | 0.69              |
| 1:K:29:GLU:HA     | 1:K:29:GLU:OE1    | 1.91                     | 0.69              |
| 1:K:39:PRO:HG3    | 1:L:39:PRO:CG     | 2.21                     | 0.69              |
| 1:L:185:ARG:HA    | 1:L:190:THR:HA    | 1.72                     | 0.69              |
| 2:M:368:THR:N     | 2:M:369:PRO:CD    | 2.55                     | 0.69              |
| 2:M:373:VAL:HG12  | 2:M:374:ASN:N     | 2.07                     | 0.69              |
| 3:N:1288:GLU:O    | 3:N:1307:LYS:HD3  | 1.92                     | 0.69              |
| 3:N:658:LEU:HD23  | 3:N:661:MET:HE1   | 1.73                     | 0.69              |
| 5:P:220:LEU:O     | 5:P:224:VAL:HG23  | 1.93                     | 0.69              |
| 1:A:70:GLY:H      | 2:C:607:ASP:HB2   | 1.57                     | 0.69              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:70:GLY:O     | 1:B:136:GLY:HA3  | 1.92                     | 0.69              |
| 2:C:492:ASP:HA   | 2:C:518:LYS:HB3  | 1.74                     | 0.69              |
| 3:D:225:LEU:HB3  | 3:D:226:PRO:HD2  | 1.73                     | 0.69              |
| 3:D:103:TRP:HZ2  | 3:D:604:THR:HG23 | 1.58                     | 0.69              |
| 1:K:183:ASP:OD2  | 2:M:938:LYS:HE3  | 1.92                     | 0.69              |
| 1:L:206:THR:HB   | 1:L:209:GLU:CD   | 2.12                     | 0.69              |
| 1:L:58:ILE:HB    | 1:L:61:VAL:HG11  | 1.75                     | 0.69              |
| 2:M:419:THR:O    | 2:M:420:ARG:HG3  | 1.93                     | 0.69              |
| 3:N:1122:LEU:O   | 3:N:1135:ARG:HG3 | 1.91                     | 0.69              |
| 3:N:1396:GLU:O   | 3:N:1398:TRP:N   | 2.23                     | 0.69              |
| 3:N:545:ARG:NE   | 5:P:257:THR:HA   | 2.07                     | 0.69              |
| 5:P:373:LYS:HB2  | 5:P:378:GLY:C    | 2.13                     | 0.69              |
| 5:P:75:ILE:HG13  | 5:P:76:SER:N     | 2.04                     | 0.69              |
| 2:C:101:ILE:CG2  | 2:C:102:HIS:H    | 2.06                     | 0.69              |
| 3:D:1038:LEU:HA  | 3:D:1061:PHE:HB2 | 1.75                     | 0.69              |
| 5:F:321:ILE:HB   | 5:F:327:SER:OG   | 1.93                     | 0.69              |
| 1:L:161:ARG:H    | 1:L:164:ALA:CB   | 2.06                     | 0.69              |
| 1:L:9:PRO:HG3    | 1:L:27:PRO:O     | 1.93                     | 0.69              |
| 1:L:92:PRO:C     | 1:L:146:ARG:HH22 | 1.96                     | 0.69              |
| 2:M:139:GLN:O    | 2:M:333:ILE:HD12 | 1.92                     | 0.69              |
| 2:M:599:GLU:HA   | 2:M:651:LYS:HB2  | 1.74                     | 0.69              |
| 3:N:1267:ARG:HE  | 3:N:1271:LYS:NZ  | 1.90                     | 0.69              |
| 3:N:173:PRO:HA   | 3:N:209:ARG:NH1  | 2.07                     | 0.69              |
| 3:N:324:ALA:HB1  | 3:N:331:VAL:HG11 | 1.74                     | 0.69              |
| 3:N:529:GLN:HB2  | 3:N:535:PHE:CD2  | 2.28                     | 0.69              |
| 1:B:217:ILE:HG22 | 1:B:221:HIS:CD2  | 2.27                     | 0.69              |
| 1:B:5:LYS:HD3    | 1:B:7:LYS:HD2    | 1.72                     | 0.69              |
| 2:C:334:ARG:HH11 | 2:C:418:LEU:HD11 | 1.58                     | 0.69              |
| 3:D:1229:ILE:O   | 3:D:1232:PRO:HD2 | 1.93                     | 0.69              |
| 3:D:1494:ALA:HB1 | 4:E:88:GLU:CB    | 2.22                     | 0.69              |
| 2:M:1052:MET:SD  | 2:M:1056:LYS:HD2 | 2.33                     | 0.69              |
| 2:M:182:VAL:HB   | 2:M:193:LEU:H    | 1.57                     | 0.69              |
| 2:M:232:GLU:HA   | 2:M:235:LEU:HD13 | 1.72                     | 0.69              |
| 2:M:672:VAL:O    | 2:M:991:GLN:HA   | 1.93                     | 0.69              |
| 3:N:1176:LYS:O   | 3:N:1179:GLU:HB2 | 1.92                     | 0.69              |
| 3:N:1196:THR:HB  | 3:N:1199:GLY:O   | 1.91                     | 0.69              |
| 3:N:241:ILE:CD1  | 3:N:310:LEU:HD22 | 2.23                     | 0.69              |
| 3:N:358:GLY:CA   | 3:N:385:VAL:HB   | 2.23                     | 0.69              |
| 3:N:680:GLN:HA   | 3:N:683:ILE:HD12 | 1.74                     | 0.69              |
| 3:N:769:LEU:N    | 3:N:769:LEU:CD1  | 2.56                     | 0.69              |
| 1:A:33:GLY:O     | 1:A:195:LEU:HD22 | 1.92                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:260:LEU:HD13  | 2:C:291:ALA:HB2   | 1.75                     | 0.69              |
| 2:C:414:GLY:N     | 2:C:419:THR:HG21  | 2.08                     | 0.69              |
| 2:C:443:THR:O     | 2:C:559:LEU:HD11  | 1.92                     | 0.69              |
| 1:A:69:PRO:HA     | 2:C:607:ASP:OD1   | 1.93                     | 0.69              |
| 3:D:353:VAL:HA    | 3:D:368:VAL:CG2   | 2.10                     | 0.69              |
| 3:D:60:CYS:HB2    | 3:D:62:LYS:HE2    | 1.75                     | 0.69              |
| 2:C:949:LYS:NZ    | 3:D:796:ARG:HH12  | 1.90                     | 0.69              |
| 3:D:819:GLY:HA2   | 3:D:824:ASN:HD22  | 1.56                     | 0.69              |
| 5:F:365:GLU:HA    | 5:F:368:VAL:HG13  | 1.72                     | 0.69              |
| 2:M:408:ARG:HG2   | 2:M:455:LEU:HB3   | 1.75                     | 0.69              |
| 2:M:553:ASP:HA    | 2:M:881:ASN:HA    | 1.74                     | 0.69              |
| 3:N:1118:ILE:CD1  | 3:N:1190:SER:HB2  | 2.22                     | 0.69              |
| 3:N:1127:GLU:HG3  | 3:N:1128:VAL:H    | 1.58                     | 0.69              |
| 3:N:1481:VAL:CG1  | 4:O:18:ARG:HA     | 2.23                     | 0.69              |
| 3:N:522:PRO:N     | 3:N:525:ARG:HH12  | 1.91                     | 0.69              |
| 3:N:660:LYS:HD2   | 3:N:693:GLU:OE2   | 1.91                     | 0.69              |
| 3:N:807:ALA:HA    | 3:N:833:GLU:HG2   | 1.74                     | 0.69              |
| 5:P:123:ASP:O     | 5:P:126:LEU:HB3   | 1.93                     | 0.69              |
| 1:B:152:PRO:HG2   | 1:B:155:LYS:HB2   | 1.73                     | 0.69              |
| 2:C:197:LEU:HB3   | 2:C:207:LEU:CD1   | 2.22                     | 0.69              |
| 2:C:276:LYS:HA    | 2:C:280:LYS:HE3   | 1.74                     | 0.69              |
| 3:D:1344:VAL:HG13 | 3:D:1345:GLU:N    | 2.07                     | 0.69              |
| 3:D:61:GLY:O      | 3:D:64:LYS:HE3    | 1.92                     | 0.69              |
| 3:D:65:ARG:HG3    | 3:D:67:ARG:H      | 1.58                     | 0.69              |
| 2:C:949:LYS:NZ    | 3:D:796:ARG:NH1   | 2.40                     | 0.69              |
| 1:L:5:LYS:HZ3     | 1:L:189:ARG:CZ    | 2.06                     | 0.69              |
| 2:M:178:PRO:O     | 2:M:220:GLY:HA2   | 1.93                     | 0.69              |
| 2:M:575:GLN:HE21  | 2:M:670:GLN:HB3   | 1.58                     | 0.69              |
| 2:M:1046:ALA:HB1  | 3:N:1471:LEU:HD11 | 1.74                     | 0.69              |
| 3:N:367:ILE:HG22  | 3:N:368:VAL:HG23  | 1.74                     | 0.69              |
| 3:N:845:ASN:HB2   | 3:N:848:GLU:CB    | 2.22                     | 0.69              |
| 3:N:87:ARG:HG3    | 3:N:88:TYR:CD2    | 2.28                     | 0.69              |
| 5:P:276:ARG:O     | 5:P:280:GLN:HG2   | 1.91                     | 0.69              |
| 5:P:321:ILE:HG13  | 5:P:332:PHE:HE1   | 1.56                     | 0.69              |
| 2:C:72:ARG:O      | 2:C:94:LEU:HD12   | 1.93                     | 0.69              |
| 2:C:926:PHE:CE2   | 2:C:960:GLU:HG3   | 2.21                     | 0.69              |
| 3:D:119:SER:N     | 3:D:123:LEU:HD12  | 2.07                     | 0.69              |
| 3:D:1377:LYS:HE2  | 3:D:1394:VAL:HG22 | 1.75                     | 0.69              |
| 3:D:264:LEU:HB2   | 3:D:267:GLY:N     | 2.07                     | 0.69              |
| 3:D:527:MET:SD    | 3:D:537:THR:HG23  | 2.34                     | 0.69              |
| 3:D:916:TYR:CZ    | 3:D:920:LEU:HD11  | 2.28                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:930:LEU:O     | 3:D:934:LEU:HG    | 1.92                     | 0.69              |
| 2:M:230:ARG:HE    | 2:M:233:GLU:CG    | 1.95                     | 0.69              |
| 2:M:327:HIS:HB3   | 2:M:330:ASN:HD22  | 1.58                     | 0.69              |
| 2:M:41:ASN:HD22   | 2:M:46:ALA:HB2    | 1.58                     | 0.69              |
| 2:M:439:CYS:CB    | 2:M:541:SER:HB3   | 2.22                     | 0.69              |
| 2:M:774:LEU:HD13  | 2:M:775:ARG:N     | 2.07                     | 0.69              |
| 3:N:1405:GLU:CD   | 3:N:1406:ARG:H    | 1.96                     | 0.69              |
| 3:N:647:ARG:O     | 3:N:650:LEU:HB3   | 1.92                     | 0.69              |
| 3:N:858:VAL:HG12  | 3:N:859:ASP:H     | 1.55                     | 0.69              |
| 5:P:159:ILE:HG22  | 5:P:163:LEU:HD11  | 1.74                     | 0.69              |
| 5:P:321:ILE:HD11  | 5:P:329:TYR:N     | 2.08                     | 0.69              |
| 1:B:10:VAL:HG22   | 1:B:26:GLU:O      | 1.93                     | 0.68              |
| 2:C:3:ILE:HG13    | 2:C:3:ILE:O       | 1.93                     | 0.68              |
| 2:C:512:ARG:HH11  | 2:C:524:VAL:HA    | 1.58                     | 0.68              |
| 5:F:291:ILE:HA    | 5:F:294:ALA:HB3   | 1.75                     | 0.68              |
| 1:L:112:ARG:HB3   | 1:L:112:ARG:NH1   | 2.08                     | 0.68              |
| 2:M:1060:ILE:HG22 | 2:M:1061:GLU:N    | 2.08                     | 0.68              |
| 2:M:1096:ALA:O    | 2:M:1097:LEU:HD23 | 1.93                     | 0.68              |
| 2:M:722:ILE:HD11  | 2:M:805:ARG:NH2   | 2.08                     | 0.68              |
| 3:N:1114:THR:HG21 | 3:N:1193:THR:O    | 1.93                     | 0.68              |
| 3:N:127:LEU:CD2   | 3:N:461:ILE:HD11  | 2.22                     | 0.68              |
| 3:N:298:VAL:HB    | 3:N:300:LYS:HE3   | 1.75                     | 0.68              |
| 3:N:673:ALA:HA    | 3:N:676:MET:HB3   | 1.74                     | 0.68              |
| 1:B:143:ARG:HD3   | 1:B:144:VAL:N     | 2.09                     | 0.68              |
| 2:C:1009:SER:HB3  | 3:D:651:GLU:OE2   | 1.93                     | 0.68              |
| 2:C:1101:THR:O    | 2:C:1102:LEU:HD23 | 1.93                     | 0.68              |
| 2:C:164:PRO:HD2   | 2:C:170:PRO:O     | 1.92                     | 0.68              |
| 2:C:145:GLY:HA3   | 2:C:276:LYS:HD2   | 1.74                     | 0.68              |
| 3:D:1367:HIS:HA   | 3:D:1370:ILE:HD12 | 1.74                     | 0.68              |
| 3:D:640:HIS:HB2   | 3:D:764:LEU:HD11  | 1.76                     | 0.68              |
| 5:F:364:ARG:O     | 5:F:368:VAL:HG13  | 1.93                     | 0.68              |
| 2:M:1091:GLU:O    | 2:M:1094:ALA:HB3  | 1.92                     | 0.68              |
| 2:M:230:ARG:N     | 2:M:230:ARG:HD3   | 2.08                     | 0.68              |
| 2:C:139:GLN:O     | 2:C:333:ILE:HD12  | 1.93                     | 0.68              |
| 2:C:269:LEU:HA    | 2:C:288:ARG:HB2   | 1.75                     | 0.68              |
| 2:C:438:ILE:HG23  | 2:C:453:THR:OG1   | 1.94                     | 0.68              |
| 3:D:107:ASP:O     | 3:D:110:SER:HA    | 1.94                     | 0.68              |
| 3:D:127:LEU:HD23  | 3:D:128:TYR:H     | 1.56                     | 0.68              |
| 3:D:680:GLN:HA    | 3:D:683:ILE:HD12  | 1.75                     | 0.68              |
| 3:D:907:GLU:O     | 3:D:911:LEU:HG    | 1.93                     | 0.68              |
| 5:F:373:LYS:HD3   | 5:F:379:ARG:HB3   | 1.74                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:K:5:LYS:NZ      | 1:K:28:LEU:C       | 2.47                     | 0.68              |
| 2:M:1096:ALA:HB1  | 3:N:13:ALA:HB3     | 1.75                     | 0.68              |
| 2:M:144:PRO:HB3   | 2:M:163:ILE:O      | 1.93                     | 0.68              |
| 2:M:260:LEU:HD12  | 2:M:288:ARG:HG2    | 1.75                     | 0.68              |
| 2:M:299:LYS:HE2   | 2:M:301:GLU:CG     | 2.23                     | 0.68              |
| 2:M:739:GLU:OE1   | 2:M:739:GLU:HA     | 1.93                     | 0.68              |
| 2:M:904:PRO:HD2   | 2:M:908:GLY:CA     | 2.23                     | 0.68              |
| 2:M:944:LEU:HD21  | 2:M:963:LEU:HD23   | 1.75                     | 0.68              |
| 2:M:838:LYS:HG3   | 2:M:997:LEU:HB2    | 1.74                     | 0.68              |
| 3:N:470:LEU:HB2   | 3:N:503:LEU:HD21   | 1.74                     | 0.68              |
| 3:N:990:ASP:HA    | 3:N:993:LEU:CD1    | 2.23                     | 0.68              |
| 2:C:289:THR:HG22  | 2:C:290:LEU:HG     | 1.75                     | 0.68              |
| 2:C:304:LEU:CB    | 2:C:305:PRO:HD3    | 2.16                     | 0.68              |
| 2:C:54:ILE:HD13   | 2:C:355:VAL:HG11   | 1.75                     | 0.68              |
| 3:D:1099:VAL:HG12 | 10:D:1529:NE6:H14B | 1.75                     | 0.68              |
| 3:D:210:ARG:HB2   | 3:D:389:GLU:CG     | 2.24                     | 0.68              |
| 3:D:794:GLN:OE1   | 3:D:794:GLN:HA     | 1.93                     | 0.68              |
| 4:E:19:LEU:O      | 4:E:23:VAL:HG23    | 1.93                     | 0.68              |
| 1:L:85:LEU:HD12   | 1:L:86:VAL:H       | 1.57                     | 0.68              |
| 2:M:292:ARG:HE    | 2:M:295:ASP:CB     | 2.05                     | 0.68              |
| 3:N:1147:ARG:HB3  | 3:N:1188:VAL:HG21  | 1.76                     | 0.68              |
| 3:N:1311:LEU:HD12 | 3:N:1312:LEU:H     | 1.57                     | 0.68              |
| 3:N:583:ASP:HB2   | 3:N:604:THR:OG1    | 1.93                     | 0.68              |
| 2:C:409:ARG:NH2   | 2:C:452:ILE:HG21   | 2.07                     | 0.68              |
| 2:C:471:TYR:CZ    | 2:C:496:ILE:HD13   | 2.28                     | 0.68              |
| 2:C:690:ILE:HG23  | 2:C:694:LEU:HD12   | 1.75                     | 0.68              |
| 2:C:773:LEU:HG    | 2:C:774:LEU:N      | 2.07                     | 0.68              |
| 3:D:227:LEU:CD1   | 3:D:326:GLU:HA     | 2.21                     | 0.68              |
| 1:K:12:THR:CA     | 1:L:229:GLN:HB3    | 2.16                     | 0.68              |
| 3:N:1041:LEU:HD11 | 3:N:1058:ARG:HA    | 1.76                     | 0.68              |
| 3:N:1126:ASP:CG   | 3:N:1129:THR:HA    | 2.13                     | 0.68              |
| 3:N:1460:ILE:HG13 | 3:N:1461:GLY:H     | 1.57                     | 0.68              |
| 3:N:188:GLY:H     | 3:N:198:ARG:HA     | 1.57                     | 0.68              |
| 3:N:260:GLU:OE1   | 3:N:273:ARG:HG3    | 1.93                     | 0.68              |
| 3:N:864:VAL:HG12  | 3:N:865:THR:N      | 2.07                     | 0.68              |
| 1:B:100:LEU:HD12  | 1:B:140:MET:O      | 1.94                     | 0.68              |
| 2:C:178:PRO:O     | 2:C:180:GLY:N      | 2.26                     | 0.68              |
| 2:C:545:ASN:O     | 2:C:581:THR:HG21   | 1.93                     | 0.68              |
| 3:D:1122:LEU:O    | 3:D:1134:LEU:HD12  | 1.94                     | 0.68              |
| 3:D:548:ILE:CG2   | 3:D:552:ASN:HD21   | 2.07                     | 0.68              |
| 3:D:546:ARG:HH21  | 3:D:577:ALA:HA     | 1.57                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:812:ALA:O    | 3:D:814:ALA:N    | 2.27                     | 0.68              |
| 2:M:72:ARG:HG2   | 2:M:95:TYR:CB    | 2.17                     | 0.68              |
| 3:N:1009:LYS:O   | 3:N:1013:GLU:HG2 | 1.93                     | 0.68              |
| 3:N:132:TYR:N    | 3:N:456:MET:HE3  | 2.09                     | 0.68              |
| 3:N:137:PRO:CD   | 3:N:453:ASP:HB3  | 2.24                     | 0.68              |
| 3:N:29:PRO:HG3   | 3:N:548:ILE:HB   | 1.76                     | 0.68              |
| 3:N:8:VAL:HG13   | 3:N:1434:TRP:CH2 | 2.29                     | 0.68              |
| 3:N:96:ALA:HB3   | 3:N:554:LEU:CD2  | 2.24                     | 0.68              |
| 5:P:78:SER:O     | 5:P:80:PRO:HD3   | 1.94                     | 0.68              |
| 2:C:1058:ASP:OD2 | 2:C:1084:SER:HB3 | 1.93                     | 0.68              |
| 2:C:205:GLU:N    | 2:C:209:ARG:HH11 | 1.92                     | 0.68              |
| 2:C:454:SER:HB3  | 2:C:541:SER:HB2  | 1.76                     | 0.68              |
| 3:D:301:GLY:C    | 3:D:303:PRO:HD2  | 2.14                     | 0.68              |
| 3:D:407:VAL:HG22 | 3:D:408:GLU:N    | 2.09                     | 0.68              |
| 2:M:380:ALA:O    | 2:M:384:GLU:N    | 2.26                     | 0.68              |
| 2:M:430:VAL:CG1  | 3:N:1075:HIS:HA  | 2.24                     | 0.68              |
| 2:M:889:HIS:ND1  | 2:M:970:GLY:HA3  | 2.08                     | 0.68              |
| 3:N:400:VAL:HG22 | 3:N:402:PRO:HD3  | 1.74                     | 0.68              |
| 3:N:701:LEU:O    | 3:N:702:LEU:HD23 | 1.94                     | 0.68              |
| 1:B:58:ILE:HD13  | 1:B:60:ASP:H     | 1.58                     | 0.68              |
| 2:C:153:ALA:O    | 2:C:155:PRO:HD3  | 1.94                     | 0.68              |
| 2:C:768:THR:HG22 | 2:C:770:GLU:H    | 1.58                     | 0.68              |
| 3:D:554:LEU:CA   | 3:D:557:LEU:HD12 | 2.20                     | 0.68              |
| 3:D:1216:SER:CB  | 4:E:16:LYS:H     | 2.06                     | 0.68              |
| 5:F:118:GLU:C    | 5:F:120:THR:H    | 1.97                     | 0.68              |
| 1:K:68:ILE:HG23  | 1:K:69:PRO:HD2   | 1.76                     | 0.68              |
| 1:L:28:LEU:HD11  | 1:L:36:LEU:HD12  | 1.74                     | 0.68              |
| 2:M:773:LEU:HD11 | 2:M:777:ILE:HD11 | 1.76                     | 0.68              |
| 2:M:964:LYS:O    | 2:M:968:LEU:HG   | 1.94                     | 0.68              |
| 3:N:142:LEU:HB3  | 3:N:146:PRO:CA   | 2.21                     | 0.68              |
| 3:N:181:ASP:C    | 3:N:183:GLU:H    | 1.97                     | 0.68              |
| 5:P:142:ARG:CD   | 5:P:145:PRO:HA   | 2.24                     | 0.68              |
| 2:C:1006:HIS:HA  | 2:C:1027:PHE:CZ  | 2.29                     | 0.68              |
| 2:C:264:PRO:HB2  | 2:C:289:THR:CG2  | 2.23                     | 0.68              |
| 2:C:1046:ALA:CB  | 3:D:1472:ILE:HB  | 2.24                     | 0.68              |
| 3:D:204:LEU:HD12 | 3:D:205:TYR:H    | 1.58                     | 0.68              |
| 3:D:482:LYS:HA   | 3:D:489:ARG:HD2  | 1.75                     | 0.68              |
| 3:D:796:ARG:C    | 3:D:797:LYS:HG2  | 2.13                     | 0.68              |
| 5:F:265:VAL:CA   | 5:F:268:ILE:HD12 | 2.23                     | 0.68              |
| 5:F:292:ALA:O    | 5:F:299:TRP:HB2  | 1.93                     | 0.68              |
| 2:M:230:ARG:HG2  | 2:M:233:GLU:HG2  | 1.76                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:341:THR:O    | 2:M:344:PHE:HB3   | 1.93                     | 0.68              |
| 3:N:837:GLY:HA2  | 3:N:841:TYR:CD1   | 2.29                     | 0.68              |
| 2:C:59:LYS:CD    | 2:C:59:LYS:H      | 2.01                     | 0.68              |
| 3:D:128:TYR:CE2  | 3:D:575:GLN:NE2   | 2.62                     | 0.68              |
| 5:F:173:TYR:HA   | 5:F:176:ILE:HD12  | 1.76                     | 0.68              |
| 5:F:107:GLU:OE1  | 5:F:230:LYS:HE3   | 1.94                     | 0.68              |
| 2:C:774:LEU:HD11 | 5:F:422:LEU:HD23  | 1.76                     | 0.68              |
| 2:M:1014:SER:HB3 | 2:M:1017:THR:OG1  | 1.94                     | 0.68              |
| 2:M:12:VAL:HG23  | 2:M:13:ILE:HG23   | 1.76                     | 0.68              |
| 3:N:812:ALA:CB   | 3:N:816:HIS:HB2   | 2.24                     | 0.68              |
| 3:N:819:GLY:HA2  | 3:N:822:ALA:HB3   | 1.76                     | 0.68              |
| 3:N:965:GLU:HG3  | 3:N:969:ARG:NH2   | 2.01                     | 0.68              |
| 5:P:300:ASP:O    | 5:P:304:VAL:HG23  | 1.93                     | 0.68              |
| 2:C:374:ASN:ND2  | 2:C:377:PRO:HD3   | 2.09                     | 0.67              |
| 3:D:1080:GLY:O   | 3:D:1084:THR:HG22 | 1.93                     | 0.67              |
| 3:D:154:THR:O    | 3:D:157:GLU:HB2   | 1.94                     | 0.67              |
| 3:D:186:VAL:HG12 | 3:D:187:LYS:N     | 2.08                     | 0.67              |
| 3:D:237:LYS:CB   | 3:D:238:PRO:HD2   | 2.16                     | 0.67              |
| 3:D:470:LEU:HB2  | 3:D:503:LEU:HD21  | 1.75                     | 0.67              |
| 1:K:138:LEU:HD12 | 1:K:139:ASN:H     | 1.59                     | 0.67              |
| 2:M:1007:ALA:HA  | 3:N:627:GLY:HA2   | 1.75                     | 0.67              |
| 2:M:203:ASP:HB2  | 2:M:228:ALA:O     | 1.94                     | 0.67              |
| 3:N:1353:GLN:OE1 | 3:N:1353:GLN:HA   | 1.92                     | 0.67              |
| 3:N:1498:ALA:HB3 | 4:O:84:ARG:NE     | 2.09                     | 0.67              |
| 3:N:219:GLU:HB3  | 3:N:337:LEU:HD12  | 1.76                     | 0.67              |
| 3:N:693:GLU:HA   | 4:O:48:MET:CE     | 2.23                     | 0.67              |
| 3:N:983:LEU:HD22 | 3:N:987:GLU:HB3   | 1.76                     | 0.67              |
| 2:C:313:LEU:C    | 2:C:315:ALA:H     | 1.98                     | 0.67              |
| 2:C:700:TYR:CB   | 2:C:833:LEU:HD22  | 2.25                     | 0.67              |
| 3:D:629:SER:C    | 3:D:744:GLN:HG2   | 2.15                     | 0.67              |
| 2:M:254:VAL:HB   | 2:M:258:TYR:CZ    | 2.29                     | 0.67              |
| 2:M:66:LEU:HA    | 2:M:99:GLN:O      | 1.94                     | 0.67              |
| 2:M:690:ILE:O    | 2:M:853:LEU:N     | 2.21                     | 0.67              |
| 3:N:1496:GLU:HA  | 3:N:1499:ARG:CB   | 2.23                     | 0.67              |
| 3:N:287:GLY:HA3  | 3:N:311:LEU:HA    | 1.76                     | 0.67              |
| 3:N:130:SER:N    | 3:N:568:ARG:NH2   | 2.43                     | 0.67              |
| 3:N:623:VAL:CG1  | 3:N:624:ASP:N     | 2.57                     | 0.67              |
| 3:N:82:LYS:H     | 3:N:82:LYS:HD2    | 1.59                     | 0.67              |
| 3:N:85:VAL:HG22  | 3:N:89:ARG:HG3    | 1.75                     | 0.67              |
| 2:C:194:VAL:HG22 | 2:C:221:LEU:HG    | 1.75                     | 0.67              |
| 2:C:694:LEU:HD21 | 2:C:868:ASP:CB    | 2.21                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1016:PRO:HA   | 3:D:1021:TYR:CD1 | 2.29                     | 0.67              |
| 3:D:135:LEU:HD23  | 3:D:135:LEU:H    | 1.57                     | 0.67              |
| 3:D:238:PRO:HB3   | 3:D:317:VAL:C    | 2.14                     | 0.67              |
| 3:D:906:GLN:HB3   | 3:D:911:LEU:HD21 | 1.77                     | 0.67              |
| 3:D:947:ILE:HG23  | 3:D:947:ILE:O    | 1.93                     | 0.67              |
| 5:F:126:LEU:O     | 5:F:129:GLU:HB3  | 1.93                     | 0.67              |
| 2:M:205:GLU:O     | 2:M:209:ARG:HB2  | 1.95                     | 0.67              |
| 3:N:230:TRP:CZ2   | 3:N:233:LYS:HE3  | 2.28                     | 0.67              |
| 3:N:223:LEU:O     | 3:N:332:TYR:HA   | 1.94                     | 0.67              |
| 5:P:407:LYS:O     | 5:P:411:HIS:HB3  | 1.94                     | 0.67              |
| 2:C:1104:GLU:H    | 2:C:1104:GLU:CD  | 1.98                     | 0.67              |
| 2:C:710:ILE:HG22  | 2:C:823:VAL:HB   | 1.75                     | 0.67              |
| 3:D:1015:TYR:N    | 3:D:1016:PRO:HD3 | 2.09                     | 0.67              |
| 3:D:534:ARG:HH21  | 5:F:313:GLU:CB   | 2.00                     | 0.67              |
| 3:D:806:PHE:CA    | 3:D:809:PRO:HD2  | 2.24                     | 0.67              |
| 3:D:96:ALA:HB3    | 3:D:554:LEU:HD23 | 1.77                     | 0.67              |
| 1:L:213:GLN:O     | 1:L:217:ILE:HG13 | 1.95                     | 0.67              |
| 1:L:226:SER:O     | 1:L:228:PRO:HD3  | 1.93                     | 0.67              |
| 2:M:958:THR:CG2   | 2:M:961:GLU:HB2  | 2.22                     | 0.67              |
| 3:N:352:ASN:O     | 3:N:368:VAL:HG13 | 1.93                     | 0.67              |
| 3:N:371:ILE:HG13  | 3:N:372:ASP:H    | 1.57                     | 0.67              |
| 3:N:401:TYR:O     | 3:N:444:VAL:HG22 | 1.95                     | 0.67              |
| 3:N:931:LEU:CA    | 3:N:934:LEU:HD12 | 2.23                     | 0.67              |
| 5:P:419:ARG:O     | 5:P:421:PHE:N    | 2.27                     | 0.67              |
| 2:C:1038:TRP:CH2  | 3:D:1096:ARG:HA  | 2.29                     | 0.67              |
| 2:C:37:GLU:HG2    | 2:C:71:TYR:CE2   | 2.29                     | 0.67              |
| 3:D:1337:GLU:N    | 3:D:1337:GLU:OE1 | 2.26                     | 0.67              |
| 3:D:133:ILE:HG22  | 3:D:455:ARG:O    | 1.95                     | 0.67              |
| 3:D:440:VAL:CG2   | 3:D:441:ARG:H    | 2.05                     | 0.67              |
| 3:D:631:ILE:HG12  | 3:D:743:ASP:O    | 1.95                     | 0.67              |
| 5:F:413:SER:CB    | 5:F:414:ARG:HH21 | 2.07                     | 0.67              |
| 2:M:94:LEU:O      | 2:M:114:PHE:HA   | 1.94                     | 0.67              |
| 2:M:95:TYR:CG     | 2:M:114:PHE:HB3  | 2.29                     | 0.67              |
| 2:M:773:LEU:CD2   | 5:P:354:LEU:HD22 | 2.24                     | 0.67              |
| 3:N:1029:ARG:HH11 | 3:N:1029:ARG:HG3 | 1.58                     | 0.67              |
| 3:N:1397:LYS:HZ3  | 3:N:1432:LYS:HD2 | 1.58                     | 0.67              |
| 5:P:159:ILE:O     | 5:P:162:LYS:HB2  | 1.95                     | 0.67              |
| 2:C:175:GLU:C     | 2:C:183:SER:HB2  | 2.15                     | 0.67              |
| 2:C:876:VAL:HA    | 2:C:881:ASN:HD21 | 1.60                     | 0.67              |
| 3:D:105:VAL:HA    | 3:D:110:SER:OG   | 1.94                     | 0.67              |
| 3:D:1498:ALA:HB2  | 4:E:87:LYS:NZ    | 2.10                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:260:GLU:H     | 3:D:270:LEU:HD12 | 1.58                     | 0.67              |
| 3:D:258:VAL:CB    | 3:D:273:ARG:HB2  | 2.09                     | 0.67              |
| 3:D:563:PRO:O     | 3:D:566:ILE:HG12 | 1.95                     | 0.67              |
| 3:D:654:LYS:HE2   | 3:D:658:LEU:HD11 | 1.75                     | 0.67              |
| 4:E:7:ASP:HA      | 4:E:10:PHE:CD1   | 2.30                     | 0.67              |
| 5:F:314:PRO:HG2   | 5:F:315:VAL:H    | 1.60                     | 0.67              |
| 1:K:188:GLN:HG3   | 1:K:189:ARG:N    | 2.05                     | 0.67              |
| 1:L:32:PHE:HA     | 1:L:35:THR:HB    | 1.76                     | 0.67              |
| 1:L:68:ILE:HD12   | 1:L:71:VAL:CG1   | 2.24                     | 0.67              |
| 2:M:1102:LEU:O    | 3:N:5:VAL:HA     | 1.93                     | 0.67              |
| 2:M:37:GLU:HG2    | 2:M:71:TYR:HE2   | 1.58                     | 0.67              |
| 2:M:918:LEU:HD12  | 2:M:968:LEU:HA   | 1.76                     | 0.67              |
| 3:N:957:PRO:HG2   | 3:N:1007:VAL:HA  | 1.77                     | 0.67              |
| 3:N:1046:GLN:HA   | 3:N:1052:THR:HA  | 1.77                     | 0.67              |
| 3:N:438:ASP:HA    | 3:N:445:ARG:NH2  | 2.09                     | 0.67              |
| 3:N:572:ARG:HH12  | 5:P:84:TYR:N     | 1.93                     | 0.67              |
| 5:P:77:THR:C      | 5:P:79:ASP:H     | 1.97                     | 0.67              |
| 2:C:395:LYS:HE2   | 2:C:403:SER:HB2  | 1.77                     | 0.67              |
| 3:D:1033:GLN:O    | 3:D:1037:GLN:HG3 | 1.93                     | 0.67              |
| 3:D:109:PRO:HB2   | 3:D:114:THR:OG1  | 1.93                     | 0.67              |
| 3:D:563:PRO:HD2   | 3:D:566:ILE:HD11 | 1.77                     | 0.67              |
| 3:D:60:CYS:SG     | 3:D:76:CYS:HB3   | 2.34                     | 0.67              |
| 2:M:254:VAL:HB    | 2:M:258:TYR:CE1  | 2.29                     | 0.67              |
| 2:M:397:GLU:N     | 2:M:633:GLN:NE2  | 2.39                     | 0.67              |
| 3:N:421:LEU:CG    | 3:N:428:LYS:HA   | 2.13                     | 0.67              |
| 5:P:333:ILE:CD1   | 5:P:333:ILE:H    | 2.08                     | 0.67              |
| 1:A:118:ALA:O     | 1:A:120:VAL:HG23 | 1.95                     | 0.67              |
| 3:D:1106:VAL:HG12 | 3:D:1107:VAL:N   | 2.10                     | 0.67              |
| 3:D:1383:ASP:HB3  | 3:D:1416:ALA:N   | 2.05                     | 0.67              |
| 3:D:234:GLU:C     | 3:D:236:TYR:H    | 1.98                     | 0.67              |
| 4:E:70:THR:C      | 4:E:72:ARG:H     | 1.98                     | 0.67              |
| 1:K:41:ARG:HG2    | 1:K:45:LEU:HD11  | 1.77                     | 0.67              |
| 3:N:1069:GLU:HA   | 3:N:1072:ILE:CD1 | 2.25                     | 0.67              |
| 3:N:1106:VAL:HG13 | 3:N:1219:GLU:O   | 1.95                     | 0.67              |
| 3:N:1337:GLU:OE1  | 3:N:1337:GLU:N   | 2.27                     | 0.67              |
| 3:N:249:TYR:CE1   | 3:N:330:THR:HG21 | 2.29                     | 0.67              |
| 3:N:593:ASN:HB3   | 3:N:594:PRO:HD3  | 1.77                     | 0.67              |
| 3:N:79:GLU:HG2    | 3:N:80:VAL:N     | 2.09                     | 0.67              |
| 1:B:208:LEU:HG    | 1:B:209:GLU:N    | 2.09                     | 0.67              |
| 2:C:474:VAL:HG12  | 2:C:530:GLU:O    | 1.94                     | 0.67              |
| 2:C:762:LYS:HB2   | 2:C:786:LYS:HD2  | 1.77                     | 0.67              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:79:PRO:HG2    | 2:C:82:GLU:CB     | 2.25                     | 0.67              |
| 2:C:857:ASP:CB    | 2:C:978:ARG:HG2   | 2.25                     | 0.67              |
| 3:D:1398:TRP:N    | 3:D:1398:TRP:CE3  | 2.61                     | 0.67              |
| 3:D:297:ILE:HD13  | 3:D:298:VAL:CG2   | 2.16                     | 0.67              |
| 3:D:334:THR:C     | 3:D:335:LEU:HD12  | 2.15                     | 0.67              |
| 3:D:217:LYS:HB2   | 3:D:339:TRP:NE1   | 2.09                     | 0.67              |
| 4:E:8:LYS:O       | 4:E:12:MET:HG3    | 1.95                     | 0.67              |
| 4:E:6:ILE:HG23    | 4:E:7:ASP:H       | 1.60                     | 0.67              |
| 2:M:670:GLN:O     | 2:M:672:VAL:HG12  | 1.95                     | 0.67              |
| 3:N:1033:GLN:N    | 3:N:1033:GLN:CD   | 2.41                     | 0.67              |
| 3:D:408:GLU:HA    | 3:D:421:LEU:O     | 1.94                     | 0.67              |
| 1:K:41:ARG:O      | 1:K:45:LEU:HG     | 1.95                     | 0.67              |
| 2:M:605:LYS:HB3   | 2:M:610:ARG:NH2   | 2.10                     | 0.67              |
| 3:N:1105:ILE:HD11 | 3:N:1374:GLN:NE2  | 2.10                     | 0.67              |
| 2:C:1089:VAL:HA   | 2:C:1092:LEU:HD12 | 1.77                     | 0.66              |
| 3:D:127:LEU:CD2   | 3:D:128:TYR:N     | 2.57                     | 0.66              |
| 3:D:430:ASP:OD1   | 3:D:430:ASP:N     | 2.28                     | 0.66              |
| 3:D:520:LEU:HD23  | 3:D:525:ARG:HB3   | 1.77                     | 0.66              |
| 3:D:819:GLY:CA    | 3:D:824:ASN:HD22  | 2.08                     | 0.66              |
| 3:D:787:LEU:HD21  | 3:D:947:ILE:HD13  | 1.76                     | 0.66              |
| 5:F:385:GLU:HA    | 5:F:388:ALA:CB    | 2.23                     | 0.66              |
| 3:N:1273:VAL:HG22 | 3:N:1326:THR:OG1  | 1.94                     | 0.66              |
| 3:N:264:LEU:HD22  | 3:N:316:GLN:HE21  | 1.60                     | 0.66              |
| 3:N:141:ILE:HD12  | 3:N:450:TYR:H     | 1.59                     | 0.66              |
| 3:N:711:LEU:HD22  | 3:N:778:LEU:CD2   | 2.25                     | 0.66              |
| 2:C:93:PRO:HA     | 2:C:117:HIS:HB3   | 1.77                     | 0.66              |
| 3:D:14:SER:HB2    | 3:D:17:LYS:HB2    | 1.77                     | 0.66              |
| 3:D:317:VAL:HG23  | 3:D:338:GLU:C     | 2.16                     | 0.66              |
| 3:D:592:THR:HG21  | 3:D:598:ARG:HH12  | 1.59                     | 0.66              |
| 3:D:644:LEU:C     | 3:D:721:VAL:HG22  | 2.16                     | 0.66              |
| 5:F:340:SER:OG    | 5:F:342:VAL:HB    | 1.95                     | 0.66              |
| 1:K:199:ILE:HB    | 1:K:207:PRO:HB3   | 1.76                     | 0.66              |
| 2:M:577:PRO:HA    | 2:M:671:ASN:OD1   | 1.96                     | 0.66              |
| 3:N:1031:ASN:CG   | 3:N:1034:GLN:HG3  | 2.14                     | 0.66              |
| 3:N:1098:LEU:HD12 | 3:N:1098:LEU:N    | 2.04                     | 0.66              |
| 3:N:1269:LYS:C    | 3:N:1271:LYS:H    | 1.97                     | 0.66              |
| 3:N:1424:VAL:HG23 | 3:N:1425:THR:N    | 2.09                     | 0.66              |
| 3:N:262:LYS:O     | 3:N:268:ALA:HA    | 1.95                     | 0.66              |
| 1:A:10:VAL:N      | 1:A:26:GLU:O      | 2.28                     | 0.66              |
| 1:A:42:ARG:NH1    | 1:B:34:VAL:HB     | 2.10                     | 0.66              |
| 2:C:219:GLN:C     | 2:C:221:LEU:H     | 1.98                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:200:LEU:HD22  | 2:C:300:ASP:HB3   | 1.78                     | 0.66              |
| 2:C:367:LEU:CG    | 2:C:372:LEU:HD21  | 2.26                     | 0.66              |
| 3:D:1083:ASP:HB2  | 3:D:1239:ARG:CZ   | 2.25                     | 0.66              |
| 3:D:245:LEU:N     | 3:D:246:PRO:HD3   | 2.09                     | 0.66              |
| 5:F:164:LYS:HA    | 5:F:171:LYS:HE3   | 1.76                     | 0.66              |
| 5:F:321:ILE:HG22  | 5:F:322:GLY:N     | 2.09                     | 0.66              |
| 5:F:347:GLN:O     | 5:F:350:LEU:HB3   | 1.96                     | 0.66              |
| 3:N:1112:CYS:H    | 3:N:1201:CYS:CB   | 2.07                     | 0.66              |
| 3:N:1237:THR:O    | 3:N:1255:GLY:HA3  | 1.96                     | 0.66              |
| 3:N:128:TYR:HD2   | 3:N:128:TYR:H     | 1.42                     | 0.66              |
| 3:N:1489:GLN:HA   | 3:N:1492:LEU:HD12 | 1.76                     | 0.66              |
| 3:N:323:GLU:CD    | 3:N:334:THR:HB    | 2.15                     | 0.66              |
| 5:P:83:GLN:O      | 5:P:86:HIS:ND1    | 2.26                     | 0.66              |
| 2:C:402:SER:HA    | 2:C:566:THR:HG23  | 1.77                     | 0.66              |
| 2:C:415:PRO:HB2   | 2:C:418:LEU:CB    | 2.23                     | 0.66              |
| 3:D:264:LEU:HD12  | 3:D:267:GLY:HA3   | 1.76                     | 0.66              |
| 3:D:736:PHE:O     | 3:D:738:ALA:N     | 2.29                     | 0.66              |
| 5:F:104:ARG:HG3   | 5:F:105:LYS:N     | 2.09                     | 0.66              |
| 2:M:349:ALA:O     | 2:M:353:ARG:HG3   | 1.95                     | 0.66              |
| 2:M:511:GLU:O     | 2:M:525:SER:HA    | 1.96                     | 0.66              |
| 2:M:498:GLN:HB2   | 2:M:514:VAL:HG23  | 1.76                     | 0.66              |
| 3:N:1384:PRO:HB3  | 3:N:1387:SER:O    | 1.95                     | 0.66              |
| 3:N:206:ARG:HG3   | 3:N:207:PHE:N     | 2.11                     | 0.66              |
| 3:N:253:ALA:H     | 3:N:301:GLY:CA    | 2.05                     | 0.66              |
| 3:N:828:LYS:HD3   | 3:N:828:LYS:H     | 1.60                     | 0.66              |
| 1:B:30:ARG:HA     | 1:B:193:ASP:OD1   | 1.95                     | 0.66              |
| 2:C:230:ARG:O     | 2:C:233:GLU:HG3   | 1.95                     | 0.66              |
| 2:C:20:GLU:O      | 2:C:23:VAL:HG22   | 1.96                     | 0.66              |
| 3:D:1094:LEU:HD21 | 3:D:1229:ILE:HG22 | 1.78                     | 0.66              |
| 3:D:175:VAL:CG1   | 3:D:192:ALA:HB1   | 2.25                     | 0.66              |
| 3:D:342:PRO:O     | 3:D:343:LYS:HG3   | 1.95                     | 0.66              |
| 3:D:367:ILE:HG22  | 3:D:368:VAL:HG23  | 1.78                     | 0.66              |
| 3:D:629:SER:HA    | 3:D:744:GLN:HE21  | 1.59                     | 0.66              |
| 5:F:279:GLN:HA    | 5:F:284:ARG:O     | 1.96                     | 0.66              |
| 5:F:396:ARG:HA    | 5:F:399:GLN:NE2   | 2.09                     | 0.66              |
| 3:N:1103:HIS:CD2  | 3:N:1462:LEU:H    | 2.13                     | 0.66              |
| 3:N:1277:ILE:HG22 | 3:N:1278:ASP:N    | 2.10                     | 0.66              |
| 3:N:252:ARG:CZ    | 3:N:300:LYS:HG2   | 2.26                     | 0.66              |
| 3:N:455:ARG:HB2   | 3:N:460:ALA:HB2   | 1.76                     | 0.66              |
| 3:N:98:PRO:HA     | 3:N:514:LEU:O     | 1.96                     | 0.66              |
| 2:C:186:VAL:CG2   | 2:C:187:ASN:N     | 2.50                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:195:LEU:CB    | 2:C:238:LEU:HD21  | 2.23                     | 0.66              |
| 2:C:292:ARG:HE    | 2:C:295:ASP:HB3   | 1.60                     | 0.66              |
| 2:C:110:GLU:CD    | 2:C:369:PRO:HB3   | 2.16                     | 0.66              |
| 3:D:1171:VAL:HG12 | 3:D:1175:ILE:HD11 | 1.75                     | 0.66              |
| 3:D:1107:VAL:HG21 | 3:D:1219:GLU:HB3  | 1.77                     | 0.66              |
| 3:D:1121:PRO:HD3  | 3:D:1346:ARG:HH21 | 1.61                     | 0.66              |
| 3:D:661:MET:SD    | 3:D:673:ALA:HB1   | 2.35                     | 0.66              |
| 2:C:988:VAL:CG1   | 3:D:948:THR:HB    | 2.23                     | 0.66              |
| 2:M:290:LEU:CD2   | 2:M:302:VAL:HG21  | 2.26                     | 0.66              |
| 2:M:909:ALA:HB1   | 2:M:914:ILE:CD1   | 2.24                     | 0.66              |
| 3:N:1406:ARG:HD3  | 3:N:1412:LYS:HZ3  | 1.57                     | 0.66              |
| 3:N:876:SER:OG    | 3:N:879:ARG:HG2   | 1.95                     | 0.66              |
| 3:N:939:PHE:O     | 3:N:942:SER:N     | 2.29                     | 0.66              |
| 4:O:46:PRO:O      | 4:O:56:ASP:HA     | 1.96                     | 0.66              |
| 2:C:867:VAL:HG23  | 2:C:868:ASP:N     | 2.09                     | 0.66              |
| 3:D:250:LEU:HD11  | 3:D:304:LEU:CD2   | 2.25                     | 0.66              |
| 3:D:522:PRO:HA    | 3:D:525:ARG:NH1   | 2.11                     | 0.66              |
| 5:F:365:GLU:O     | 5:F:368:VAL:HG22  | 1.94                     | 0.66              |
| 1:L:124:ASN:ND2   | 1:L:127:LEU:HD22  | 2.11                     | 0.66              |
| 2:M:87:ASP:HA     | 2:M:131:GLY:HA3   | 1.76                     | 0.66              |
| 3:N:154:THR:HG22  | 3:N:157:GLU:HG3   | 1.76                     | 0.66              |
| 3:N:244:GLU:O     | 3:N:246:PRO:CD    | 2.38                     | 0.66              |
| 3:N:568:ARG:HA    | 3:N:571:LYS:HD2   | 1.78                     | 0.66              |
| 3:N:812:ALA:CA    | 3:N:816:HIS:HB2   | 2.26                     | 0.66              |
| 3:N:989:TYR:HA    | 3:N:992:ILE:HD12  | 1.77                     | 0.66              |
| 3:N:99:ALA:O      | 3:N:514:LEU:N     | 2.28                     | 0.66              |
| 2:C:136:ILE:HD13  | 2:C:392:SER:HA    | 1.76                     | 0.66              |
| 2:C:162:ILE:HD12  | 2:C:172:ILE:CD1   | 2.26                     | 0.66              |
| 3:D:175:VAL:HG13  | 3:D:193:PRO:HD2   | 1.76                     | 0.66              |
| 3:D:219:GLU:HG2   | 3:D:220:ARG:H     | 1.59                     | 0.66              |
| 3:D:327:GLU:HG3   | 3:D:327:GLU:O     | 1.95                     | 0.66              |
| 3:D:414:ARG:HD3   | 3:D:451:ASP:OD1   | 1.95                     | 0.66              |
| 3:D:711:LEU:HD22  | 3:D:778:LEU:HD23  | 1.78                     | 0.66              |
| 3:D:82:LYS:HD2    | 3:D:82:LYS:H      | 1.61                     | 0.66              |
| 3:D:83:SER:OG     | 5:F:337:HIS:NE2   | 2.29                     | 0.66              |
| 1:K:186:LEU:HD23  | 1:K:188:GLN:NE2   | 2.10                     | 0.66              |
| 1:K:42:ARG:HH12   | 1:L:34:VAL:HB     | 1.60                     | 0.66              |
| 1:L:104:GLU:CB    | 1:L:137:ARG:HG3   | 2.22                     | 0.66              |
| 2:M:194:VAL:HG21  | 2:M:221:LEU:O     | 1.94                     | 0.66              |
| 2:M:595:LEU:HD21  | 2:M:639:GLN:NE2   | 2.10                     | 0.66              |
| 3:N:137:PRO:CG    | 3:N:138:LYS:H     | 2.09                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:149:LYS:HG2  | 3:N:150:ARG:N     | 2.10                     | 0.66              |
| 3:N:154:THR:O    | 3:N:157:GLU:HB2   | 1.95                     | 0.66              |
| 3:N:179:VAL:C    | 3:N:181:ASP:H     | 1.99                     | 0.66              |
| 3:N:264:LEU:HB2  | 3:N:267:GLY:N     | 2.11                     | 0.66              |
| 3:N:623:VAL:HG12 | 3:N:624:ASP:N     | 2.10                     | 0.66              |
| 3:N:643:GLY:HA3  | 3:N:727:GLN:HB2   | 1.76                     | 0.66              |
| 2:M:988:VAL:HG12 | 3:N:948:THR:OG1   | 1.95                     | 0.66              |
| 5:P:111:GLU:HA   | 5:P:114:LYS:HD2   | 1.77                     | 0.66              |
| 5:P:288:TYR:CE1  | 5:P:305:GLU:HB2   | 2.31                     | 0.66              |
| 2:C:672:VAL:HG23 | 2:C:868:ASP:OD2   | 1.95                     | 0.66              |
| 3:D:133:ILE:HG23 | 3:D:456:MET:CG    | 2.25                     | 0.66              |
| 3:D:1103:HIS:HD2 | 3:D:1463:LYS:H    | 1.43                     | 0.66              |
| 3:D:172:PRO:HB2  | 3:D:175:VAL:CG2   | 2.26                     | 0.66              |
| 3:D:258:VAL:H    | 3:D:273:ARG:N     | 1.93                     | 0.66              |
| 3:D:397:LYS:HE3  | 3:D:448:GLU:OE2   | 1.96                     | 0.66              |
| 5:F:371:LEU:HD23 | 5:F:375:LEU:HD11  | 1.75                     | 0.66              |
| 2:M:403:SER:O    | 2:M:406:HIS:HB3   | 1.96                     | 0.66              |
| 2:M:397:GLU:HG2  | 2:M:632:ASN:HB2   | 1.77                     | 0.66              |
| 2:M:720:GLU:HB3  | 2:M:760:SER:HB3   | 1.78                     | 0.66              |
| 3:N:1124:GLN:N   | 3:N:1133:ARG:O    | 2.27                     | 0.66              |
| 3:N:1464:GLU:O   | 3:N:1467:ILE:HG22 | 1.95                     | 0.66              |
| 3:N:674:ARG:NH2  | 5:P:342:VAL:HG22  | 2.11                     | 0.66              |
| 3:N:887:ALA:HA   | 3:N:890:VAL:HG22  | 1.77                     | 0.66              |
| 1:A:143:ARG:NH1  | 1:A:158:ILE:HG23  | 2.11                     | 0.66              |
| 1:B:239:ALA:O    | 1:B:241:GLU:N     | 2.28                     | 0.66              |
| 2:C:191:PHE:CE2  | 2:C:196:LEU:HD21  | 2.30                     | 0.66              |
| 2:C:243:ARG:CG   | 2:C:244:PRO:HA    | 2.26                     | 0.66              |
| 2:C:38:LYS:CG    | 2:C:39:ARG:H      | 2.07                     | 0.66              |
| 2:C:436:GLY:HA2  | 2:C:539:VAL:HA    | 1.76                     | 0.66              |
| 2:C:754:ILE:HG12 | 2:C:791:ARG:CD    | 2.26                     | 0.66              |
| 2:C:676:ILE:CG2  | 2:C:988:VAL:HG13  | 2.25                     | 0.66              |
| 3:D:1144:LEU:HA  | 3:D:1147:ARG:HG3  | 1.77                     | 0.66              |
| 3:D:109:PRO:HB2  | 3:D:114:THR:HG21  | 1.76                     | 0.66              |
| 3:D:1399:ASP:O   | 3:D:1403:LEU:HB3  | 1.96                     | 0.66              |
| 3:D:248:PRO:HA   | 3:D:308:LYS:NZ    | 2.10                     | 0.66              |
| 3:D:259:VAL:HG23 | 3:D:270:LEU:HD13  | 1.78                     | 0.66              |
| 3:D:474:GLU:HG2  | 3:D:475:LYS:N     | 2.10                     | 0.66              |
| 1:L:156:HIS:CG   | 1:L:156:HIS:O     | 2.49                     | 0.66              |
| 2:M:232:GLU:O    | 2:M:235:LEU:HB3   | 1.96                     | 0.66              |
| 2:M:419:THR:HG22 | 2:M:420:ARG:N     | 2.11                     | 0.66              |
| 2:M:428:ARG:CZ   | 2:M:451:LEU:HD21  | 2.25                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:876:VAL:H     | 2:M:877:PRO:HD2   | 1.60                     | 0.66              |
| 3:N:1267:ARG:NH1  | 3:N:1267:ARG:CB   | 2.54                     | 0.66              |
| 3:N:592:THR:HG21  | 3:N:598:ARG:HH12  | 1.60                     | 0.66              |
| 3:N:614:PHE:HA    | 3:N:617:ASN:HD22  | 1.60                     | 0.66              |
| 2:C:402:SER:HA    | 2:C:566:THR:CG2   | 2.26                     | 0.65              |
| 2:C:724:ARG:HH21  | 2:C:734:LEU:CB    | 2.09                     | 0.65              |
| 2:C:674:VAL:HA    | 2:C:869:VAL:HG13  | 1.78                     | 0.65              |
| 2:C:889:HIS:CD2   | 2:C:970:GLY:HA3   | 2.31                     | 0.65              |
| 2:C:987:ILE:HA    | 3:D:948:THR:CG2   | 2.25                     | 0.65              |
| 3:D:1397:LYS:HB2  | 3:D:1398:TRP:CE3  | 2.31                     | 0.65              |
| 3:D:365:ASP:O     | 3:D:379:ALA:HB2   | 1.96                     | 0.65              |
| 3:D:455:ARG:HD3   | 3:D:459:GLU:CD    | 2.16                     | 0.65              |
| 3:D:545:ARG:HH11  | 3:D:545:ARG:HB3   | 1.61                     | 0.65              |
| 1:L:161:ARG:H     | 1:L:164:ALA:HB2   | 1.60                     | 0.65              |
| 2:M:649:VAL:HG13  | 2:M:650:ARG:NH2   | 2.10                     | 0.65              |
| 3:N:153:LEU:HD21  | 3:N:158:TYR:HA    | 1.78                     | 0.65              |
| 3:N:325:GLU:O     | 3:N:325:GLU:HG3   | 1.96                     | 0.65              |
| 3:N:133:ILE:HD13  | 3:N:456:MET:HE1   | 1.78                     | 0.65              |
| 3:N:553:ARG:HH11  | 5:P:214:GLN:CB    | 2.08                     | 0.65              |
| 3:N:565:ILE:HG12  | 3:N:566:ILE:N     | 2.11                     | 0.65              |
| 5:P:274:THR:HG22  | 5:P:278:LEU:HD11  | 1.77                     | 0.65              |
| 3:N:207:PHE:CE1   | 5:P:98:GLU:HG3    | 2.31                     | 0.65              |
| 2:C:170:PRO:HD3   | 2:C:263:ASP:HB3   | 1.77                     | 0.65              |
| 2:C:197:LEU:CD1   | 2:C:221:LEU:HD11  | 2.25                     | 0.65              |
| 2:C:274:ARG:O     | 2:C:278:GLU:HB3   | 1.96                     | 0.65              |
| 2:C:712:ALA:HB3   | 2:C:821:GLU:H     | 1.61                     | 0.65              |
| 3:D:1102:THR:O    | 3:D:1222:GLY:HA3  | 1.96                     | 0.65              |
| 3:D:1311:LEU:CD1  | 3:D:1312:LEU:H    | 2.09                     | 0.65              |
| 3:D:615:ARG:HG3   | 3:D:616:GLN:N     | 2.11                     | 0.65              |
| 2:C:988:VAL:H     | 3:D:948:THR:HG21  | 1.61                     | 0.65              |
| 5:F:173:TYR:O     | 5:F:176:ILE:HB    | 1.96                     | 0.65              |
| 1:K:154:GLU:H     | 1:K:154:GLU:CD    | 1.98                     | 0.65              |
| 2:M:216:GLU:OE2   | 2:M:217:LEU:HG    | 1.95                     | 0.65              |
| 3:N:1085:ALA:CA   | 3:N:1088:THR:HG22 | 2.26                     | 0.65              |
| 3:N:115:LEU:O     | 3:N:116:LEU:HD23  | 1.96                     | 0.65              |
| 3:N:1459:LEU:HD12 | 3:N:1470:ARG:NH1  | 2.10                     | 0.65              |
| 3:N:257:GLY:CA    | 3:N:274:ARG:HA    | 2.26                     | 0.65              |
| 3:N:630:VAL:HA    | 3:N:744:GLN:HG2   | 1.78                     | 0.65              |
| 3:N:22:SER:CB     | 3:N:92:HIS:ND1    | 2.59                     | 0.65              |
| 4:O:41:GLU:HB2    | 4:O:42:PRO:CD     | 2.20                     | 0.65              |
| 5:P:392:VAL:CG1   | 5:P:396:ARG:HB3   | 2.26                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:18:ARG:O     | 1:B:207:PRO:HD3   | 1.97                     | 0.65              |
| 1:B:216:GLU:OE2  | 1:B:220:GLU:HB2   | 1.97                     | 0.65              |
| 1:B:69:PRO:O     | 1:B:71:VAL:HG23   | 1.95                     | 0.65              |
| 2:C:456:ALA:HB1  | 2:C:538:GLN:O     | 1.97                     | 0.65              |
| 3:D:168:THR:HB   | 3:D:206:ARG:NH2   | 2.12                     | 0.65              |
| 3:D:356:PRO:HG2  | 3:D:359:ALA:HB2   | 1.78                     | 0.65              |
| 3:D:403:PHE:CZ   | 3:D:442:ASN:HB3   | 2.29                     | 0.65              |
| 3:D:539:ASP:HB3  | 3:D:600:LEU:HB3   | 1.78                     | 0.65              |
| 1:L:137:ARG:HG2  | 1:L:137:ARG:HH11  | 1.60                     | 0.65              |
| 2:M:198:ARG:HA   | 2:M:202:TYR:O     | 1.97                     | 0.65              |
| 2:M:204:GLN:C    | 2:M:209:ARG:HD3   | 2.17                     | 0.65              |
| 3:N:1400:VAL:HB  | 3:N:1401:GLU:OE1  | 1.96                     | 0.65              |
| 3:N:1468:LEU:CD2 | 3:N:1469:GLY:N    | 2.60                     | 0.65              |
| 3:N:315:ARG:HD2  | 3:N:315:ARG:H     | 1.60                     | 0.65              |
| 3:N:403:PHE:HB2  | 3:N:423:ASP:OD2   | 1.96                     | 0.65              |
| 5:P:153:PRO:HG2  | 5:P:154:LYS:HG3   | 1.77                     | 0.65              |
| 5:P:330:GLY:O    | 5:P:332:PHE:N     | 2.30                     | 0.65              |
| 1:A:108:GLU:HG2  | 1:A:109:VAL:H     | 1.59                     | 0.65              |
| 2:C:742:VAL:HG12 | 2:C:743:VAL:N     | 2.11                     | 0.65              |
| 2:C:70:GLU:OE1   | 2:C:97:ARG:HD3    | 1.96                     | 0.65              |
| 3:D:166:GLN:O    | 3:D:167:GLU:HG2   | 1.96                     | 0.65              |
| 3:D:352:ASN:O    | 3:D:368:VAL:HG13  | 1.97                     | 0.65              |
| 3:D:441:ARG:HD3  | 3:D:443:VAL:HG21  | 1.78                     | 0.65              |
| 3:D:526:PRO:O    | 3:D:537:THR:HG22  | 1.95                     | 0.65              |
| 5:F:353:GLU:HA   | 5:F:356:LYS:HD2   | 1.79                     | 0.65              |
| 2:M:1086:ARG:HB3 | 2:M:1112:PHE:CE2  | 2.30                     | 0.65              |
| 2:M:186:VAL:HG13 | 2:M:187:ASN:N     | 2.08                     | 0.65              |
| 2:M:293:PHE:CD1  | 2:M:294:GLU:HG3   | 2.31                     | 0.65              |
| 2:M:305:PRO:O    | 2:M:308:ARG:HG2   | 1.95                     | 0.65              |
| 2:M:542:VAL:HG23 | 2:M:543:ASN:N     | 2.06                     | 0.65              |
| 2:M:930:LYS:C    | 2:M:932:GLU:H     | 2.00                     | 0.65              |
| 3:N:207:PHE:CE1  | 5:P:97:GLU:HB2    | 2.31                     | 0.65              |
| 3:N:212:ARG:HD3  | 3:N:342:PRO:CB    | 2.26                     | 0.65              |
| 5:P:234:LYS:HE2  | 5:P:236:SER:CB    | 2.26                     | 0.65              |
| 5:P:263:HIS:HA   | 5:P:266:GLU:OE2   | 1.97                     | 0.65              |
| 1:A:86:VAL:HG13  | 1:A:123:MET:HB2   | 1.77                     | 0.65              |
| 1:B:74:ASP:HB3   | 1:B:77:GLU:CB     | 2.27                     | 0.65              |
| 2:C:257:VAL:HG12 | 2:C:263:ASP:OD1   | 1.96                     | 0.65              |
| 2:C:1:MET:HB3    | 2:C:898:GLY:O     | 1.97                     | 0.65              |
| 3:D:1083:ASP:HB2 | 3:D:1239:ARG:NH1  | 2.12                     | 0.65              |
| 3:D:1341:PRO:O   | 3:D:1344:VAL:HG12 | 1.97                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1376:MET:HE1 | 3:D:1421:LEU:HD13 | 1.78                     | 0.65              |
| 3:D:414:ARG:HD3  | 3:D:451:ASP:CG    | 2.17                     | 0.65              |
| 3:D:851:LEU:O    | 3:D:854:ALA:HB3   | 1.96                     | 0.65              |
| 3:D:881:LEU:HG   | 3:D:885:ILE:HD11  | 1.79                     | 0.65              |
| 5:F:217:ASN:O    | 5:F:220:LEU:HB3   | 1.96                     | 0.65              |
| 5:F:76:SER:O     | 5:F:78:SER:N      | 2.28                     | 0.65              |
| 2:M:203:ASP:O    | 2:M:207:LEU:HD12  | 1.96                     | 0.65              |
| 2:M:367:LEU:HD23 | 2:M:367:LEU:O     | 1.96                     | 0.65              |
| 3:N:1342:GLU:HA  | 3:N:1345:GLU:OE1  | 1.97                     | 0.65              |
| 3:N:524:LEU:C    | 3:N:526:PRO:HD3   | 2.17                     | 0.65              |
| 1:A:186:LEU:HD23 | 1:A:188:GLN:HE21  | 1.60                     | 0.65              |
| 1:A:5:LYS:HZ2    | 1:A:28:LEU:C      | 2.00                     | 0.65              |
| 1:B:137:ARG:HH11 | 1:B:137:ARG:HG2   | 1.61                     | 0.65              |
| 2:C:370:ALA:HA   | 2:C:373:VAL:CG2   | 2.25                     | 0.65              |
| 2:C:405:ARG:HD2  | 2:C:442:GLU:OE2   | 1.96                     | 0.65              |
| 2:C:672:VAL:HG23 | 2:C:673:LEU:N     | 2.11                     | 0.65              |
| 3:D:288:MET:CE   | 3:D:307:ALA:HB2   | 2.26                     | 0.65              |
| 3:D:354:VAL:HB   | 3:D:367:ILE:O     | 1.97                     | 0.65              |
| 3:D:965:GLU:O    | 3:D:968:ASP:N     | 2.30                     | 0.65              |
| 4:E:42:PRO:HA    | 4:E:45:ARG:HD2    | 1.77                     | 0.65              |
| 5:F:373:LYS:HB3  | 5:F:379:ARG:N     | 2.11                     | 0.65              |
| 1:K:41:ARG:NH2   | 2:M:860:HIS:CD2   | 2.64                     | 0.65              |
| 2:M:498:GLN:OE1  | 3:N:1067:VAL:HG13 | 1.95                     | 0.65              |
| 2:M:435:TYR:HA   | 3:N:1071:PHE:CE2  | 2.32                     | 0.65              |
| 3:N:207:PHE:HZ   | 5:P:98:GLU:HG3    | 1.62                     | 0.65              |
| 2:C:205:GLU:O    | 2:C:209:ARG:HB2   | 1.96                     | 0.65              |
| 2:C:45:GLN:O     | 2:C:49:ARG:HG3    | 1.97                     | 0.65              |
| 2:C:56:GLU:HB3   | 2:C:359:MET:SD    | 2.36                     | 0.65              |
| 3:D:1098:LEU:CD1 | 3:D:1098:LEU:H    | 2.10                     | 0.65              |
| 3:D:610:LYS:HZ3  | 3:D:1442:ASN:H    | 1.44                     | 0.65              |
| 3:D:225:LEU:HD12 | 3:D:333:LEU:CD1   | 2.26                     | 0.65              |
| 3:D:252:ARG:HG3  | 3:D:300:LYS:C     | 2.17                     | 0.65              |
| 5:F:207:LEU:O    | 5:F:212:LEU:HD21  | 1.96                     | 0.65              |
| 5:F:280:GLN:CG   | 5:F:281:GLU:H     | 1.95                     | 0.65              |
| 2:M:151:ASP:HB3  | 2:M:157:ARG:O     | 1.97                     | 0.65              |
| 2:M:153:ALA:O    | 2:M:155:PRO:HD3   | 1.96                     | 0.65              |
| 3:N:1108:ARG:CD  | 3:N:1199:GLY:HA3  | 2.26                     | 0.65              |
| 3:N:148:GLU:O    | 3:N:150:ARG:N     | 2.29                     | 0.65              |
| 3:N:274:ARG:HE   | 3:N:279:VAL:CG1   | 2.08                     | 0.65              |
| 4:O:37:ASN:HD22  | 4:O:37:ASN:N      | 1.93                     | 0.65              |
| 5:P:302:LYS:HD2  | 5:P:302:LYS:C     | 2.17                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1030:GLN:O    | 3:D:622:ARG:HA    | 1.97                     | 0.65              |
| 2:C:508:ILE:HD12  | 2:C:526:PRO:HB3   | 1.79                     | 0.65              |
| 2:C:643:VAL:HG23  | 2:C:647:GLN:CD    | 2.17                     | 0.65              |
| 3:D:1042:ARG:HH11 | 3:D:1042:ARG:HG2  | 1.62                     | 0.65              |
| 3:D:1406:ARG:HA   | 3:D:1412:LYS:HG2  | 1.78                     | 0.65              |
| 3:D:238:PRO:HD3   | 3:D:318:ARG:HA    | 1.77                     | 0.65              |
| 3:D:811:GLU:HB2   | 3:D:816:HIS:ND1   | 2.11                     | 0.65              |
| 1:L:5:LYS:HZ1     | 1:L:189:ARG:HD2   | 1.61                     | 0.65              |
| 1:L:86:VAL:HG13   | 1:L:123:MET:HB2   | 1.78                     | 0.65              |
| 3:N:1313:VAL:HG22 | 3:N:1314:LYS:N    | 2.12                     | 0.65              |
| 3:N:441:ARG:O     | 3:N:443:VAL:N     | 2.30                     | 0.65              |
| 1:B:101:LEU:HB3   | 1:B:140:MET:SD    | 2.37                     | 0.65              |
| 3:D:249:TYR:CD1   | 3:D:330:THR:HG21  | 2.32                     | 0.65              |
| 3:D:259:VAL:CA    | 3:D:270:LEU:HD11  | 2.27                     | 0.65              |
| 3:D:245:LEU:HA    | 3:D:309:GLY:H     | 1.62                     | 0.65              |
| 3:D:315:ARG:H     | 3:D:315:ARG:HD2   | 1.62                     | 0.65              |
| 3:D:647:ARG:O     | 3:D:650:LEU:HB3   | 1.97                     | 0.65              |
| 3:D:673:ALA:HA    | 3:D:676:MET:HB3   | 1.78                     | 0.65              |
| 3:D:56:TYR:OH     | 3:D:82:LYS:HE3    | 1.97                     | 0.65              |
| 5:F:421:PHE:CD2   | 5:F:422:LEU:N     | 2.65                     | 0.65              |
| 3:N:166:GLN:HA    | 3:N:395:VAL:O     | 1.96                     | 0.65              |
| 3:N:131:LYS:HB3   | 3:N:568:ARG:HG2   | 1.77                     | 0.65              |
| 3:N:625:TYR:HB3   | 3:N:749:VAL:HB    | 1.79                     | 0.65              |
| 3:N:959:GLU:H     | 3:N:959:GLU:CD    | 2.00                     | 0.65              |
| 3:N:962:GLN:HB3   | 3:N:966:GLU:OE2   | 1.96                     | 0.65              |
| 5:P:367:MET:CB    | 5:P:371:LEU:HG    | 2.27                     | 0.65              |
| 5:P:94:LEU:CG     | 5:P:190:ALA:HB1   | 2.26                     | 0.65              |
| 1:A:83:LYS:HE3    | 1:A:168:ASP:O     | 1.96                     | 0.65              |
| 2:C:1115:LEU:HB3  | 3:D:85:VAL:CG2    | 2.21                     | 0.65              |
| 3:D:128:TYR:HD1   | 3:D:457:GLY:CA    | 2.08                     | 0.65              |
| 3:D:12:LEU:HD21   | 3:D:1452:ILE:HD13 | 1.78                     | 0.65              |
| 3:D:400:VAL:HG23  | 3:D:443:VAL:CG1   | 2.27                     | 0.65              |
| 3:D:887:ALA:HA    | 3:D:890:VAL:CG2   | 2.27                     | 0.65              |
| 2:M:41:ASN:ND2    | 2:M:41:ASN:C      | 2.49                     | 0.65              |
| 2:M:45:GLN:O      | 2:M:49:ARG:HG3    | 1.96                     | 0.65              |
| 2:M:914:ILE:N     | 2:M:914:ILE:HD12  | 2.11                     | 0.65              |
| 3:N:1122:LEU:C    | 3:N:1135:ARG:HG3  | 2.17                     | 0.65              |
| 3:N:1175:ILE:O    | 3:N:1179:GLU:HG3  | 1.97                     | 0.65              |
| 3:N:1406:ARG:HG2  | 3:N:1412:LYS:HD3  | 1.79                     | 0.65              |
| 3:N:174:GLY:HA2   | 3:N:389:GLU:CG    | 2.27                     | 0.65              |
| 3:N:544:TYR:O     | 3:N:547:LEU:HB3   | 1.97                     | 0.65              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:931:LEU:HA    | 3:N:934:LEU:CD1   | 2.27                     | 0.65              |
| 3:N:972:LEU:HD23  | 3:N:972:LEU:N     | 2.12                     | 0.65              |
| 5:P:413:SER:HB2   | 5:P:414:ARG:HH21  | 1.61                     | 0.65              |
| 1:B:176:ARG:HG2   | 1:B:177:VAL:N     | 2.12                     | 0.64              |
| 2:C:328:LEU:HD12  | 2:C:433:THR:O     | 1.97                     | 0.64              |
| 2:C:685:GLU:O     | 2:C:686:ASP:HB2   | 1.95                     | 0.64              |
| 2:C:425:PHE:HZ    | 3:D:1239:ARG:NH2  | 1.94                     | 0.64              |
| 3:D:1403:LEU:C    | 3:D:1405:GLU:H    | 2.01                     | 0.64              |
| 3:D:546:ARG:O     | 3:D:550:ARG:HG3   | 1.97                     | 0.64              |
| 3:D:58:CYS:HB2    | 3:D:76:CYS:SG     | 2.37                     | 0.64              |
| 4:E:70:THR:O      | 4:E:72:ARG:N      | 2.30                     | 0.64              |
| 5:F:213:ILE:HG22  | 5:F:217:ASN:HD21  | 1.62                     | 0.64              |
| 5:F:271:LEU:HD11  | 5:F:307:THR:HG21  | 1.78                     | 0.64              |
| 2:M:313:LEU:C     | 2:M:315:ALA:H     | 2.00                     | 0.64              |
| 2:M:600:ASP:HA    | 2:M:649:VAL:O     | 1.97                     | 0.64              |
| 3:N:1120:VAL:HB   | 3:N:1144:LEU:HD21 | 1.79                     | 0.64              |
| 3:N:1403:LEU:HB3  | 3:N:1408:ILE:CD1  | 2.27                     | 0.64              |
| 3:N:261:LEU:HD22  | 3:N:268:ALA:O     | 1.97                     | 0.64              |
| 2:C:1037:VAL:HG21 | 10:D:1529:NE6:H9  | 1.79                     | 0.64              |
| 2:C:836:GLY:O     | 2:C:848:VAL:HG13  | 1.97                     | 0.64              |
| 3:D:1472:ILE:HG23 | 3:D:1474:ALA:H    | 1.61                     | 0.64              |
| 3:D:280:ALA:HB1   | 3:D:282:TYR:CE1   | 2.32                     | 0.64              |
| 3:D:421:LEU:HB3   | 3:D:427:VAL:O     | 1.97                     | 0.64              |
| 3:D:659:LYS:HG3   | 3:D:663:GLU:OE2   | 1.96                     | 0.64              |
| 1:K:89:PHE:HB2    | 1:K:146:ARG:HH21  | 1.63                     | 0.64              |
| 2:M:172:ILE:HG22  | 2:M:173:ASP:N     | 2.12                     | 0.64              |
| 2:M:613:VAL:O     | 2:M:620:LEU:HA    | 1.97                     | 0.64              |
| 3:N:149:LYS:HG2   | 3:N:150:ARG:H     | 1.63                     | 0.64              |
| 3:N:352:ASN:N     | 3:N:369:ALA:O     | 2.31                     | 0.64              |
| 3:N:537:THR:C     | 5:P:317:LEU:HG    | 2.17                     | 0.64              |
| 2:M:1009:SER:HB3  | 3:N:651:GLU:CD    | 2.17                     | 0.64              |
| 3:N:965:GLU:OE2   | 3:N:969:ARG:HB3   | 1.96                     | 0.64              |
| 1:A:208:LEU:HG    | 1:A:209:GLU:N     | 2.11                     | 0.64              |
| 2:C:139:GLN:HB3   | 2:C:411:SER:HB3   | 1.80                     | 0.64              |
| 2:C:809:GLY:C     | 2:C:811:PRO:HD2   | 2.18                     | 0.64              |
| 3:D:10:ILE:O      | 3:D:1454:GLY:HA2  | 1.97                     | 0.64              |
| 3:D:1121:PRO:CD   | 3:D:1346:ARG:HH21 | 2.10                     | 0.64              |
| 3:D:417:PRO:HB3   | 3:D:429:SER:C     | 2.18                     | 0.64              |
| 3:D:524:LEU:C     | 3:D:526:PRO:HD3   | 2.18                     | 0.64              |
| 3:D:793:THR:O     | 3:D:905:PRO:HA    | 1.96                     | 0.64              |
| 4:E:73:LEU:HD12   | 4:E:74:VAL:H      | 1.61                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:145:PRO:O    | 5:F:149:GLU:HB2   | 1.97                     | 0.64              |
| 1:K:33:GLY:HA3   | 1:K:181:VAL:HG22  | 1.79                     | 0.64              |
| 1:L:170:VAL:O    | 1:L:170:VAL:HG23  | 1.96                     | 0.64              |
| 2:M:1009:SER:HB3 | 3:N:651:GLU:OE2   | 1.97                     | 0.64              |
| 2:M:896:PHE:C    | 2:M:898:GLY:N     | 2.50                     | 0.64              |
| 3:N:113:GLY:C    | 3:N:115:LEU:H     | 2.01                     | 0.64              |
| 3:N:1147:ARG:HB3 | 3:N:1188:VAL:CG2  | 2.27                     | 0.64              |
| 3:N:1114:THR:HB  | 3:N:1195:GLN:CG   | 2.27                     | 0.64              |
| 3:N:1293:PHE:CZ  | 3:N:1300:SER:HB3  | 2.32                     | 0.64              |
| 3:N:1324:PRO:O   | 3:N:1325:LEU:HD23 | 1.98                     | 0.64              |
| 3:N:225:LEU:HB3  | 3:N:226:PRO:HD2   | 1.78                     | 0.64              |
| 3:N:96:ALA:HB3   | 3:N:554:LEU:HD23  | 1.79                     | 0.64              |
| 3:N:699:VAL:HG12 | 3:N:717:GLN:CG    | 2.26                     | 0.64              |
| 3:N:852:ALA:HB1  | 3:N:857:ILE:HD11  | 1.78                     | 0.64              |
| 3:N:25:GLU:HB2   | 3:N:92:HIS:CE1    | 2.33                     | 0.64              |
| 5:P:219:GLY:HA3  | 5:P:246:ALA:CB    | 2.27                     | 0.64              |
| 5:P:299:TRP:CE3  | 5:P:303:ARG:HD3   | 2.32                     | 0.64              |
| 1:A:56:VAL:HG22  | 1:A:142:VAL:HA    | 1.78                     | 0.64              |
| 1:A:167:VAL:HG12 | 1:A:168:ASP:N     | 2.11                     | 0.64              |
| 1:B:68:ILE:HD12  | 1:B:71:VAL:HB     | 1.79                     | 0.64              |
| 1:B:72:LYS:HD3   | 1:B:72:LYS:C      | 2.17                     | 0.64              |
| 1:B:82:LEU:O     | 1:B:85:LEU:HB3    | 1.97                     | 0.64              |
| 2:C:140:ILE:HG23 | 2:C:410:ILE:CG2   | 2.27                     | 0.64              |
| 2:C:469:THR:HG23 | 2:C:470:PRO:HD2   | 1.80                     | 0.64              |
| 2:C:470:PRO:HG3  | 2:C:485:TYR:CZ    | 2.32                     | 0.64              |
| 2:C:705:ILE:HD12 | 2:C:705:ILE:N     | 2.13                     | 0.64              |
| 2:C:815:LEU:HD11 | 2:C:821:GLU:HA    | 1.79                     | 0.64              |
| 2:C:939:ARG:HD2  | 2:C:982:PRO:CD    | 2.28                     | 0.64              |
| 3:D:1333:HIS:O   | 3:D:1336:LEU:HB3  | 1.98                     | 0.64              |
| 3:D:142:LEU:HD23 | 3:D:146:PRO:CA    | 2.27                     | 0.64              |
| 3:D:298:VAL:O    | 3:D:298:VAL:HG12  | 1.97                     | 0.64              |
| 3:D:212:ARG:HG3  | 3:D:343:LYS:O     | 1.98                     | 0.64              |
| 3:D:806:PHE:CD1  | 3:D:809:PRO:HB2   | 2.31                     | 0.64              |
| 3:D:815:ALA:HA   | 3:D:818:ARG:CD    | 2.27                     | 0.64              |
| 3:D:785:ILE:HD13 | 3:D:935:LYS:HA    | 1.79                     | 0.64              |
| 5:F:339:PRO:HB3  | 5:F:343:ASP:HB2   | 1.78                     | 0.64              |
| 5:F:346:THR:O    | 5:F:350:LEU:N     | 2.31                     | 0.64              |
| 2:M:495:THR:HB   | 2:M:530:GLU:HG3   | 1.80                     | 0.64              |
| 2:M:672:VAL:CG2  | 2:M:673:LEU:N     | 2.61                     | 0.64              |
| 2:M:71:TYR:HD2   | 2:M:71:TYR:N      | 1.95                     | 0.64              |
| 2:M:93:PRO:HA    | 2:M:117:HIS:CB    | 2.24                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1106:VAL:HG12 | 3:N:1107:VAL:N    | 2.13                     | 0.64              |
| 3:N:1130:ARG:HH22 | 3:N:1323:GLN:NE2  | 1.94                     | 0.64              |
| 3:N:112:ILE:HG23  | 3:N:512:MET:SD    | 2.38                     | 0.64              |
| 3:N:818:ARG:O     | 3:N:822:ALA:N     | 2.27                     | 0.64              |
| 3:N:844:ALA:HB1   | 3:N:867:ARG:HH11  | 1.61                     | 0.64              |
| 1:A:206:THR:HB    | 1:A:209:GLU:CG    | 2.18                     | 0.64              |
| 2:C:693:GLU:HG3   | 2:C:697:ARG:HH11  | 1.63                     | 0.64              |
| 3:D:1031:ASN:N    | 3:D:1034:GLN:HE21 | 1.96                     | 0.64              |
| 2:C:878:SER:HA    | 3:D:1034:GLN:OE1  | 1.98                     | 0.64              |
| 3:D:227:LEU:HD22  | 3:D:328:GLY:C     | 2.18                     | 0.64              |
| 3:D:355:VAL:HG11  | 3:D:385:VAL:CG2   | 2.24                     | 0.64              |
| 3:D:125:GLN:HE22  | 3:D:587:ARG:HE    | 1.45                     | 0.64              |
| 1:K:55:SER:HB3    | 1:K:166:PRO:HA    | 1.78                     | 0.64              |
| 2:M:41:ASN:O      | 2:M:46:ALA:HB2    | 1.97                     | 0.64              |
| 3:N:119:SER:HB3   | 3:N:123:LEU:CG    | 2.27                     | 0.64              |
| 3:N:1258:ARG:NE   | 3:N:1262:LEU:HD11 | 2.13                     | 0.64              |
| 3:N:302:GLN:N     | 3:N:303:PRO:HD2   | 2.12                     | 0.64              |
| 3:N:403:PHE:CD1   | 3:N:404:GLU:N     | 2.65                     | 0.64              |
| 3:N:163:TYR:OH    | 5:P:186:HIS:HE1   | 1.81                     | 0.64              |
| 1:A:11:PHE:HD2    | 1:B:227:ASN:O     | 1.80                     | 0.64              |
| 2:C:95:TYR:CD2    | 2:C:114:PHE:HB3   | 2.32                     | 0.64              |
| 2:C:363:SER:CB    | 2:C:366:SER:HB3   | 2.21                     | 0.64              |
| 2:C:37:GLU:OE2    | 2:C:70:GLU:HB3    | 1.98                     | 0.64              |
| 3:D:1396:GLU:O    | 3:D:1397:LYS:HD3  | 1.98                     | 0.64              |
| 3:D:1406:ARG:HB3  | 3:D:1412:LYS:HE2  | 1.79                     | 0.64              |
| 3:D:815:ALA:HA    | 3:D:818:ARG:HD2   | 1.79                     | 0.64              |
| 3:D:851:LEU:N     | 3:D:851:LEU:HD23  | 2.12                     | 0.64              |
| 5:F:278:LEU:HB3   | 5:F:286:PRO:HG3   | 1.80                     | 0.64              |
| 5:F:381:HIS:C     | 5:F:385:GLU:HG3   | 2.17                     | 0.64              |
| 2:M:760:SER:O     | 2:M:785:VAL:HA    | 1.98                     | 0.64              |
| 3:N:433:GLY:CA    | 3:N:449:SER:N     | 2.60                     | 0.64              |
| 3:N:807:ALA:N     | 3:N:809:PRO:HD2   | 2.12                     | 0.64              |
| 2:M:1015:LEU:HA   | 5:P:335:ASP:HB2   | 1.78                     | 0.64              |
| 2:C:230:ARG:NH1   | 2:C:230:ARG:HG3   | 2.12                     | 0.64              |
| 3:D:658:LEU:HA    | 3:D:661:MET:CE    | 2.17                     | 0.64              |
| 2:C:971:LYS:NZ    | 3:D:950:GLY:HA3   | 2.13                     | 0.64              |
| 5:F:300:ASP:O     | 5:F:304:VAL:HG23  | 1.98                     | 0.64              |
| 2:M:1007:ALA:HB2  | 3:N:648:MET:HG3   | 1.78                     | 0.64              |
| 2:M:191:PHE:CE2   | 2:M:196:LEU:HD21  | 2.32                     | 0.64              |
| 2:M:100:LEU:HD23  | 2:M:368:THR:HA    | 1.80                     | 0.64              |
| 2:M:649:VAL:CA    | 2:M:650:ARG:HH21  | 2.08                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:34:VAL:HG21  | 2:M:939:ARG:HH21 | 1.62                     | 0.64              |
| 3:N:1114:THR:HB  | 3:N:1195:GLN:HG3 | 1.80                     | 0.64              |
| 3:N:1434:TRP:O   | 3:N:1437:ALA:HB3 | 1.97                     | 0.64              |
| 5:P:302:LYS:HD2  | 5:P:303:ARG:H    | 1.55                     | 0.64              |
| 2:C:549:PHE:CD2  | 2:C:886:LEU:HB2  | 2.32                     | 0.64              |
| 2:C:897:LEU:O    | 2:C:899:GLN:HG2  | 1.98                     | 0.64              |
| 2:C:904:PRO:HD2  | 2:C:908:GLY:HA2  | 1.78                     | 0.64              |
| 3:D:260:GLU:H    | 3:D:270:LEU:CD1  | 2.10                     | 0.64              |
| 3:D:437:VAL:HG11 | 5:F:175:HIS:CB   | 2.21                     | 0.64              |
| 3:D:574:LEU:O    | 3:D:578:VAL:HG23 | 1.98                     | 0.64              |
| 3:D:800:LYS:O    | 3:D:830:ALA:HB3  | 1.98                     | 0.64              |
| 5:F:115:LYS:HD2  | 5:F:119:ILE:HD11 | 1.79                     | 0.64              |
| 5:F:209:PHE:O    | 5:F:213:ILE:HG13 | 1.98                     | 0.64              |
| 2:M:317:VAL:N    | 2:M:318:PRO:CD   | 2.61                     | 0.64              |
| 2:M:317:VAL:O    | 2:M:317:VAL:HG12 | 1.98                     | 0.64              |
| 2:M:63:GLY:H     | 2:M:103:LYS:CA   | 2.10                     | 0.64              |
| 2:M:698:ASP:HA   | 2:M:832:LYS:CE   | 2.28                     | 0.64              |
| 3:N:157:GLU:O    | 3:N:161:LEU:HG   | 1.97                     | 0.64              |
| 3:N:507:ASN:ND2  | 3:N:1452:ILE:O   | 2.31                     | 0.64              |
| 3:N:680:GLN:HA   | 3:N:683:ILE:CD1  | 2.27                     | 0.64              |
| 3:N:793:THR:HG21 | 3:N:906:GLN:HG2  | 1.79                     | 0.64              |
| 2:C:194:VAL:HA   | 2:C:197:LEU:CG   | 2.28                     | 0.64              |
| 2:C:380:ALA:C    | 2:C:384:GLU:HG2  | 2.18                     | 0.64              |
| 3:D:1031:ASN:N   | 3:D:1034:GLN:NE2 | 2.44                     | 0.64              |
| 3:D:1364:HIS:ND1 | 3:D:1366:LYS:HG3 | 2.12                     | 0.64              |
| 3:D:1464:GLU:CG  | 3:D:1465:ASN:H   | 2.10                     | 0.64              |
| 3:D:826:PRO:O    | 3:D:829:VAL:HG22 | 1.97                     | 0.64              |
| 3:D:87:ARG:HB3   | 3:D:523:ASP:HB2  | 1.79                     | 0.64              |
| 1:K:34:VAL:HB    | 1:L:42:ARG:NH1   | 2.12                     | 0.64              |
| 2:M:1008:ARG:NH1 | 2:M:1020:PRO:HB3 | 2.13                     | 0.64              |
| 3:N:1372:VAL:HA  | 3:N:1375:MET:HE2 | 1.79                     | 0.64              |
| 3:N:1464:GLU:CG  | 3:N:1465:ASN:H   | 2.10                     | 0.64              |
| 4:O:25:LYS:HA    | 4:O:28:GLN:CD    | 2.17                     | 0.64              |
| 5:P:152:ASP:N    | 5:P:153:PRO:HD2  | 2.13                     | 0.64              |
| 5:P:370:LYS:O    | 5:P:375:LEU:N    | 2.30                     | 0.64              |
| 2:C:52:PHE:HE1   | 2:C:66:LEU:HG    | 1.63                     | 0.64              |
| 2:C:584:GLU:H    | 2:C:584:GLU:CD   | 2.00                     | 0.64              |
| 3:D:1310:ARG:HD3 | 3:D:1327:ARG:HD3 | 1.78                     | 0.64              |
| 3:D:168:THR:HB   | 3:D:206:ARG:HH22 | 1.62                     | 0.64              |
| 3:D:569:ASN:O    | 3:D:573:MET:HG3  | 1.97                     | 0.64              |
| 4:E:39:VAL:HG11  | 4:E:72:ARG:O     | 1.97                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:300:ASP:O     | 5:F:303:ARG:HB3   | 1.97                     | 0.64              |
| 1:L:76:VAL:HA     | 1:L:79:ILE:CD1    | 2.21                     | 0.64              |
| 2:M:1000:MET:HB2  | 2:M:1003:ASP:HB2  | 1.79                     | 0.64              |
| 2:M:439:CYS:SG    | 2:M:441:VAL:HG13  | 2.38                     | 0.64              |
| 3:N:209:ARG:O     | 3:N:346:ARG:HA    | 1.98                     | 0.64              |
| 3:N:479:GLU:C     | 3:N:481:MET:H     | 2.01                     | 0.64              |
| 3:N:656:PHE:HZ    | 3:N:751:LEU:HD23  | 1.62                     | 0.64              |
| 3:N:761:ILE:HD12  | 4:O:20:THR:HA     | 1.80                     | 0.64              |
| 3:N:796:ARG:HE    | 3:N:861:GLN:CB    | 2.11                     | 0.64              |
| 5:P:261:PRO:O     | 5:P:264:MET:HB2   | 1.97                     | 0.64              |
| 5:P:383:LEU:HD21  | 5:P:394:ARG:HD3   | 1.80                     | 0.64              |
| 1:B:197:LEU:HD12  | 1:B:198:ARG:H     | 1.63                     | 0.63              |
| 1:B:208:LEU:O     | 1:B:211:LEU:HB3   | 1.98                     | 0.63              |
| 2:C:605:LYS:CB    | 2:C:610:ARG:HH21  | 2.09                     | 0.63              |
| 3:D:676:MET:HG3   | 3:D:677:LEU:CD2   | 2.28                     | 0.63              |
| 4:E:47:LYS:O      | 4:E:48:MET:HG3    | 1.96                     | 0.63              |
| 5:F:251:ILE:O     | 5:F:255:ALA:HB2   | 1.98                     | 0.63              |
| 5:F:305:GLU:O     | 5:F:308:LEU:HG    | 1.97                     | 0.63              |
| 1:L:47:SER:C      | 1:L:48:ILE:HD12   | 2.18                     | 0.63              |
| 2:M:1113:GLU:O    | 2:M:1113:GLU:HG3  | 1.97                     | 0.63              |
| 2:M:56:GLU:O      | 2:M:64:LEU:HD23   | 1.98                     | 0.63              |
| 3:N:989:TYR:CE1   | 3:N:993:LEU:HD21  | 2.33                     | 0.63              |
| 5:P:209:PHE:O     | 5:P:213:ILE:HG13  | 1.97                     | 0.63              |
| 1:A:36:LEU:O      | 1:A:40:LEU:HD12   | 1.98                     | 0.63              |
| 3:D:109:PRO:HB2   | 3:D:114:THR:CG2   | 2.28                     | 0.63              |
| 3:D:241:ILE:HG22  | 3:D:242:LEU:N     | 2.11                     | 0.63              |
| 5:F:292:ALA:HB1   | 5:F:299:TRP:O     | 1.98                     | 0.63              |
| 1:K:228:PRO:O     | 1:K:229:GLN:HG3   | 1.97                     | 0.63              |
| 1:L:70:GLY:O      | 1:L:133:GLU:HG2   | 1.98                     | 0.63              |
| 2:M:1058:ASP:OD2  | 2:M:1084:SER:CB   | 2.45                     | 0.63              |
| 2:M:243:ARG:CG    | 2:M:244:PRO:HA    | 2.24                     | 0.63              |
| 2:M:48:PHE:CE1    | 2:M:71:TYR:HB3    | 2.32                     | 0.63              |
| 2:M:710:ILE:HD13  | 2:M:790:LEU:HB2   | 1.79                     | 0.63              |
| 3:N:1083:ASP:OD2  | 3:N:1238:MET:HB3  | 1.97                     | 0.63              |
| 3:N:1367:HIS:O    | 3:N:1371:VAL:HG23 | 1.97                     | 0.63              |
| 5:P:265:VAL:CA    | 5:P:268:ILE:HD12  | 2.25                     | 0.63              |
| 2:C:101:ILE:CG2   | 2:C:102:HIS:N     | 2.61                     | 0.63              |
| 2:C:1115:LEU:HD13 | 3:D:85:VAL:CB     | 2.24                     | 0.63              |
| 2:C:144:PRO:HB2   | 2:C:266:ARG:HB3   | 1.80                     | 0.63              |
| 2:C:38:LYS:HG3    | 2:C:39:ARG:N      | 2.07                     | 0.63              |
| 2:C:676:ILE:HG13  | 2:C:873:PRO:HG3   | 1.81                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:855:VAL:O     | 2:C:858:MET:HB3   | 1.98                     | 0.63              |
| 3:D:1108:ARG:HE   | 3:D:1199:GLY:HA3  | 1.62                     | 0.63              |
| 3:D:1120:VAL:HB   | 3:D:1144:LEU:HD21 | 1.81                     | 0.63              |
| 3:D:1206:GLY:O    | 3:D:1215:VAL:HG12 | 1.97                     | 0.63              |
| 3:D:1381:VAL:HG13 | 3:D:1389:LEU:HA   | 1.80                     | 0.63              |
| 3:D:154:THR:HG22  | 3:D:157:GLU:HG3   | 1.80                     | 0.63              |
| 5:F:322:GLY:O     | 5:F:324:GLU:HG3   | 1.97                     | 0.63              |
| 2:M:1035:MET:O    | 2:M:1038:TRP:HB2  | 1.97                     | 0.63              |
| 2:M:1040:LEU:HD23 | 3:N:763:MET:CE    | 2.28                     | 0.63              |
| 2:M:212:GLY:HA3   | 2:M:218:VAL:HG11  | 1.80                     | 0.63              |
| 2:M:588:VAL:HG23  | 2:M:589:ARG:N     | 2.12                     | 0.63              |
| 3:N:186:VAL:HA    | 3:N:200:ASP:OD2   | 1.98                     | 0.63              |
| 3:N:402:PRO:HA    | 3:N:443:VAL:HA    | 1.80                     | 0.63              |
| 3:N:402:PRO:CG    | 3:N:443:VAL:HG22  | 2.29                     | 0.63              |
| 1:A:109:VAL:HB    | 1:A:130:ALA:H     | 1.63                     | 0.63              |
| 2:C:1100:GLN:HB3  | 3:D:9:ARG:HB3     | 1.80                     | 0.63              |
| 2:C:260:LEU:HD13  | 2:C:291:ALA:CB    | 2.28                     | 0.63              |
| 2:C:292:ARG:HH21  | 2:C:295:ASP:CG    | 2.01                     | 0.63              |
| 3:D:1486:VAL:HG22 | 4:E:75:PHE:HB3    | 1.80                     | 0.63              |
| 3:D:968:ASP:O     | 3:D:972:LEU:HD23  | 1.98                     | 0.63              |
| 5:F:413:SER:HA    | 5:F:416:ARG:NH1   | 2.14                     | 0.63              |
| 1:L:58:ILE:O      | 1:L:61:VAL:HG13   | 1.98                     | 0.63              |
| 2:M:211:LEU:C     | 2:M:213:ALA:H     | 1.99                     | 0.63              |
| 2:M:480:THR:HG22  | 2:M:482:GLU:N     | 2.12                     | 0.63              |
| 2:M:694:LEU:HD21  | 2:M:868:ASP:CB    | 2.28                     | 0.63              |
| 3:N:1486:VAL:HA   | 4:O:75:PHE:HA     | 1.80                     | 0.63              |
| 3:N:358:GLY:HA2   | 3:N:385:VAL:CB    | 2.28                     | 0.63              |
| 3:N:397:LYS:HE3   | 3:N:448:GLU:OE2   | 1.98                     | 0.63              |
| 3:N:566:ILE:HA    | 3:N:569:ASN:HB3   | 1.81                     | 0.63              |
| 5:P:76:SER:O      | 5:P:78:SER:N      | 2.26                     | 0.63              |
| 1:B:70:GLY:O      | 1:B:133:GLU:HG2   | 1.99                     | 0.63              |
| 1:B:197:LEU:HD12  | 1:B:198:ARG:N     | 2.14                     | 0.63              |
| 2:C:176:VAL:HG12  | 2:C:181:VAL:O     | 1.99                     | 0.63              |
| 2:C:367:LEU:HG    | 2:C:372:LEU:HD11  | 1.81                     | 0.63              |
| 3:D:119:SER:O     | 3:D:121:THR:N     | 2.31                     | 0.63              |
| 3:D:187:LYS:HG3   | 3:D:198:ARG:CG    | 2.27                     | 0.63              |
| 3:D:210:ARG:N     | 3:D:389:GLU:HB2   | 2.14                     | 0.63              |
| 3:D:528:VAL:O     | 3:D:535:PHE:HB3   | 1.98                     | 0.63              |
| 3:D:960:LYS:HG2   | 3:D:964:LEU:CD1   | 2.28                     | 0.63              |
| 1:K:101:LEU:HD12  | 1:K:102:LYS:N     | 2.12                     | 0.63              |
| 1:K:5:LYS:HZ2     | 1:K:28:LEU:C      | 2.02                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:328:LEU:HG   | 2:M:433:THR:HB   | 1.79                     | 0.63              |
| 2:M:394:PHE:HB3  | 2:M:632:ASN:ND2  | 2.14                     | 0.63              |
| 3:N:1151:ARG:C   | 3:N:1162:GLU:HB3 | 2.18                     | 0.63              |
| 3:N:1254:GLN:HG2 | 3:N:1255:GLY:N   | 2.13                     | 0.63              |
| 3:N:1256:LEU:HB3 | 3:N:1257:PRO:HD3 | 1.80                     | 0.63              |
| 3:N:441:ARG:O    | 3:N:443:VAL:HG23 | 1.99                     | 0.63              |
| 3:N:671:LYS:CA   | 3:N:674:ARG:HB2  | 2.28                     | 0.63              |
| 1:B:117:VAL:HG12 | 1:B:118:ALA:N    | 2.12                     | 0.63              |
| 2:C:135:VAL:HG23 | 2:C:395:LYS:HA   | 1.79                     | 0.63              |
| 2:C:174:LEU:HD21 | 2:C:184:MET:HG2  | 1.80                     | 0.63              |
| 2:C:232:GLU:O    | 2:C:236:ILE:HG13 | 1.98                     | 0.63              |
| 2:C:542:VAL:CG2  | 2:C:543:ASN:H    | 2.07                     | 0.63              |
| 3:D:22:SER:HA    | 3:D:90:MET:O     | 1.98                     | 0.63              |
| 3:D:442:ASN:N    | 3:D:442:ASN:HD22 | 1.96                     | 0.63              |
| 2:M:63:GLY:H     | 2:M:103:LYS:HA   | 1.61                     | 0.63              |
| 2:M:198:ARG:HE   | 2:M:231:PRO:HD3  | 1.64                     | 0.63              |
| 2:M:217:LEU:C    | 2:M:219:GLN:H    | 2.02                     | 0.63              |
| 2:M:941:VAL:HG12 | 2:M:945:ARG:HH21 | 1.62                     | 0.63              |
| 3:N:172:PRO:O    | 3:N:175:VAL:HG23 | 1.98                     | 0.63              |
| 3:N:227:LEU:HD12 | 3:N:331:VAL:CG2  | 2.29                     | 0.63              |
| 3:N:501:ALA:O    | 3:N:505:SER:CB   | 2.46                     | 0.63              |
| 2:M:776:SER:CB   | 5:P:379:ARG:HH22 | 2.11                     | 0.63              |
| 1:B:206:THR:HG22 | 1:B:208:LEU:HB3  | 1.81                     | 0.63              |
| 2:C:211:LEU:O    | 2:C:213:ALA:N    | 2.31                     | 0.63              |
| 2:C:343:GLN:O    | 2:C:346:VAL:HG22 | 1.99                     | 0.63              |
| 2:C:578:VAL:HG23 | 2:C:579:VAL:HG12 | 1.80                     | 0.63              |
| 2:C:649:VAL:HG13 | 2:C:653:ASP:CB   | 2.29                     | 0.63              |
| 3:D:113:GLY:C    | 3:D:115:LEU:N    | 2.50                     | 0.63              |
| 3:D:259:VAL:HG23 | 3:D:270:LEU:CD1  | 2.28                     | 0.63              |
| 3:D:550:ARG:NH1  | 3:D:573:MET:HB3  | 2.14                     | 0.63              |
| 2:M:148:PHE:N    | 2:M:323:ASP:OD2  | 2.31                     | 0.63              |
| 2:M:468:ARG:HA   | 2:M:486:MET:O    | 1.99                     | 0.63              |
| 2:M:853:LEU:HB2  | 2:M:858:MET:HE3  | 1.81                     | 0.63              |
| 3:N:772:PRO:HG3  | 3:N:1210:SER:CB  | 2.27                     | 0.63              |
| 3:N:531:ASP:O    | 3:N:533:GLY:N    | 2.32                     | 0.63              |
| 3:N:811:GLU:HB2  | 3:N:816:HIS:ND1  | 2.14                     | 0.63              |
| 3:N:819:GLY:HA2  | 3:N:824:ASN:ND2  | 2.14                     | 0.63              |
| 3:N:92:HIS:HA    | 3:N:519:VAL:HG23 | 1.81                     | 0.63              |
| 1:B:152:PRO:HG2  | 1:B:155:LYS:HB3  | 1.80                     | 0.63              |
| 2:C:176:VAL:CG1  | 2:C:182:VAL:HA   | 2.29                     | 0.63              |
| 2:C:178:PRO:O    | 2:C:179:ASN:C    | 2.36                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:193:LEU:CD1  | 2:C:196:LEU:HD12  | 2.29                     | 0.63              |
| 2:C:380:ALA:O    | 2:C:384:GLU:HG2   | 1.99                     | 0.63              |
| 2:C:520:GLU:O    | 2:C:522:VAL:HG23  | 1.98                     | 0.63              |
| 2:C:987:ILE:HG23 | 3:D:948:THR:CG2   | 2.28                     | 0.63              |
| 3:D:1403:LEU:HG  | 3:D:1408:ILE:HG13 | 1.80                     | 0.63              |
| 3:D:274:ARG:NH2  | 3:D:279:VAL:HG13  | 2.13                     | 0.63              |
| 3:D:434:ARG:HD3  | 3:D:449:SER:HB3   | 1.80                     | 0.63              |
| 3:D:592:THR:HG21 | 3:D:598:ARG:NH1   | 2.14                     | 0.63              |
| 1:K:78:ILE:O     | 1:K:81:ASN:HB2    | 1.98                     | 0.63              |
| 1:L:5:LYS:HE2    | 1:L:189:ARG:NH1   | 2.13                     | 0.63              |
| 2:M:34:VAL:N     | 2:M:35:PRO:CD     | 2.61                     | 0.63              |
| 2:M:380:ALA:C    | 2:M:384:GLU:HG2   | 2.19                     | 0.63              |
| 2:M:504:GLU:O    | 2:M:506:ASN:N     | 2.32                     | 0.63              |
| 2:M:726:ILE:C    | 2:M:728:HIS:H     | 2.01                     | 0.63              |
| 3:N:849:ALA:O    | 3:N:852:ALA:HB3   | 1.98                     | 0.63              |
| 4:O:73:LEU:HD12  | 4:O:74:VAL:H      | 1.64                     | 0.63              |
| 5:P:138:SER:HA   | 5:P:141:VAL:HG13  | 1.81                     | 0.63              |
| 1:A:106:PRO:HD3  | 1:A:134:GLU:OE1   | 1.99                     | 0.63              |
| 2:C:184:MET:HG3  | 2:C:193:LEU:CD1   | 2.28                     | 0.63              |
| 2:C:199:VAL:HG21 | 2:C:238:LEU:CD1   | 2.29                     | 0.63              |
| 3:D:1107:VAL:CG2 | 3:D:1219:GLU:HB3  | 2.29                     | 0.63              |
| 3:D:119:SER:CB   | 3:D:122:GLU:HB2   | 2.28                     | 0.63              |
| 3:D:1372:VAL:HA  | 3:D:1375:MET:HE2  | 1.80                     | 0.63              |
| 3:D:178:LEU:HG   | 3:D:181:ASP:HB2   | 1.81                     | 0.63              |
| 3:D:182:GLY:HA2  | 3:D:203:ALA:CB    | 2.19                     | 0.63              |
| 3:D:127:LEU:CD2  | 3:D:461:ILE:HD11  | 2.28                     | 0.63              |
| 3:D:55:ASP:OD1   | 3:D:83:SER:N      | 2.32                     | 0.63              |
| 4:E:42:PRO:HA    | 4:E:45:ARG:CD     | 2.28                     | 0.63              |
| 4:E:85:LEU:HD23  | 4:E:85:LEU:H      | 1.63                     | 0.63              |
| 1:L:110:LYS:HD2  | 1:L:126:ASP:HA    | 1.80                     | 0.63              |
| 2:M:328:LEU:CD1  | 2:M:437:ARG:HD2   | 2.29                     | 0.63              |
| 2:M:726:ILE:CD1  | 2:M:728:HIS:HB2   | 2.29                     | 0.63              |
| 3:N:125:GLN:HG2  | 5:P:75:ILE:O      | 1.98                     | 0.63              |
| 3:N:1397:LYS:C   | 3:N:1398:TRP:CD1  | 2.72                     | 0.63              |
| 3:N:814:ALA:O    | 3:N:818:ARG:HG3   | 1.99                     | 0.63              |
| 5:P:164:LYS:HA   | 5:P:171:LYS:HE3   | 1.81                     | 0.63              |
| 1:B:215:VAL:CG2  | 1:B:216:GLU:N     | 2.62                     | 0.62              |
| 2:C:322:VAL:HG12 | 2:C:323:ASP:H     | 1.63                     | 0.62              |
| 2:C:56:GLU:HB2   | 2:C:64:LEU:CD2    | 2.29                     | 0.62              |
| 2:C:894:GLY:HA2  | 2:C:897:LEU:HB2   | 1.81                     | 0.62              |
| 3:D:644:LEU:HD12 | 3:D:645:PRO:CD    | 2.28                     | 0.62              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:875:THR:HG22  | 3:D:879:ARG:HG3   | 1.81                     | 0.62              |
| 3:D:907:GLU:OE2   | 3:D:910:SER:HB3   | 1.99                     | 0.62              |
| 3:D:962:GLN:HB3   | 3:D:966:GLU:OE2   | 1.99                     | 0.62              |
| 1:K:186:LEU:O     | 1:K:188:GLN:HG2   | 1.99                     | 0.62              |
| 1:L:91:ASN:HB3    | 1:L:94:LEU:CG     | 2.26                     | 0.62              |
| 2:M:158:TYR:CE1   | 2:M:313:LEU:HG    | 2.33                     | 0.62              |
| 2:M:89:THR:HG23   | 2:M:129:ILE:HA    | 1.81                     | 0.62              |
| 2:M:939:ARG:O     | 2:M:943:VAL:HG23  | 1.99                     | 0.62              |
| 3:N:1091:SER:C    | 3:N:1093:TYR:N    | 2.46                     | 0.62              |
| 3:N:131:LYS:HB3   | 3:N:131:LYS:HZ3   | 1.62                     | 0.62              |
| 3:N:212:ARG:HA    | 3:N:343:LYS:O     | 1.99                     | 0.62              |
| 3:N:85:VAL:HG22   | 3:N:89:ARG:CG     | 2.29                     | 0.62              |
| 2:C:1100:GLN:HA   | 2:C:1100:GLN:NE2  | 2.14                     | 0.62              |
| 2:C:649:VAL:HG22  | 2:C:650:ARG:NH2   | 2.14                     | 0.62              |
| 2:C:695:LEU:O     | 2:C:698:ASP:N     | 2.29                     | 0.62              |
| 2:C:1010:THR:HA   | 3:D:624:ASP:OD1   | 1.97                     | 0.62              |
| 5:F:382:THR:HG22  | 5:F:394:ARG:HB2   | 1.82                     | 0.62              |
| 1:K:208:LEU:HG    | 1:K:212:ASN:HD21  | 1.64                     | 0.62              |
| 1:L:156:HIS:O     | 1:L:158:ILE:N     | 2.32                     | 0.62              |
| 2:M:353:ARG:O     | 2:M:357:GLU:HG3   | 1.99                     | 0.62              |
| 2:M:979:THR:C     | 2:M:981:GLU:H     | 2.02                     | 0.62              |
| 3:N:1400:VAL:HG12 | 3:N:1404:ASN:ND2  | 2.13                     | 0.62              |
| 3:N:690:ALA:O     | 3:N:693:GLU:HB3   | 1.98                     | 0.62              |
| 3:N:921:ARG:HH11  | 3:N:921:ARG:HB3   | 1.63                     | 0.62              |
| 4:O:37:ASN:N      | 4:O:37:ASN:ND2    | 2.46                     | 0.62              |
| 3:N:1498:ALA:HB3  | 4:O:84:ARG:NH2    | 2.13                     | 0.62              |
| 5:P:339:PRO:HB3   | 5:P:343:ASP:HB2   | 1.80                     | 0.62              |
| 1:A:57:TYR:HE1    | 1:A:163:ASN:HB2   | 1.65                     | 0.62              |
| 2:C:218:VAL:O     | 2:C:218:VAL:HG22  | 1.98                     | 0.62              |
| 2:C:221:LEU:HD23  | 2:C:222:MET:HG3   | 1.81                     | 0.62              |
| 2:C:260:LEU:HB2   | 2:C:291:ALA:HB2   | 1.81                     | 0.62              |
| 3:D:1324:PRO:O    | 3:D:1325:LEU:HD23 | 1.98                     | 0.62              |
| 3:D:1330:ILE:HD12 | 3:D:1347:TYR:CE1  | 2.34                     | 0.62              |
| 3:D:318:ARG:HG2   | 3:D:319:ALA:N     | 2.14                     | 0.62              |
| 3:D:417:PRO:HG2   | 3:D:428:LYS:HE2   | 1.81                     | 0.62              |
| 3:D:798:GLU:HG3   | 3:D:799:LYS:N     | 2.14                     | 0.62              |
| 1:K:31:GLY:N      | 1:K:193:ASP:OD2   | 2.32                     | 0.62              |
| 1:L:66:SER:HB2    | 1:L:75:VAL:HG21   | 1.80                     | 0.62              |
| 2:M:265:ARG:HG3   | 2:M:265:ARG:O     | 1.98                     | 0.62              |
| 3:N:1341:PRO:O    | 3:N:1342:GLU:C    | 2.35                     | 0.62              |
| 3:N:1342:GLU:CD   | 3:N:1342:GLU:H    | 2.01                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1396:GLU:C    | 3:N:1398:TRP:H    | 2.02                     | 0.62              |
| 3:N:173:PRO:HG3   | 3:N:209:ARG:NH1   | 2.15                     | 0.62              |
| 3:N:410:SER:CB    | 5:P:178:ARG:HG3   | 2.29                     | 0.62              |
| 3:N:452:ILE:HD12  | 3:N:452:ILE:O     | 1.99                     | 0.62              |
| 3:N:45:PHE:HB3    | 3:N:86:ARG:HH22   | 1.64                     | 0.62              |
| 3:N:552:ASN:HA    | 3:N:555:LYS:HD2   | 1.81                     | 0.62              |
| 3:N:576:GLU:HA    | 3:N:579:ASP:OD2   | 1.99                     | 0.62              |
| 5:P:92:PRO:O      | 5:P:94:LEU:N      | 2.31                     | 0.62              |
| 2:C:1100:GLN:CG   | 2:C:1102:LEU:HD21 | 2.28                     | 0.62              |
| 2:C:810:ASP:N     | 2:C:811:PRO:CD    | 2.62                     | 0.62              |
| 3:D:1211:MET:HB2  | 3:D:1213:ARG:NH1  | 2.15                     | 0.62              |
| 3:D:629:SER:CA    | 3:D:744:GLN:HE21  | 2.13                     | 0.62              |
| 3:D:849:ALA:O     | 3:D:852:ALA:HB3   | 1.98                     | 0.62              |
| 4:E:6:ILE:O       | 4:E:9:LEU:HB2     | 1.99                     | 0.62              |
| 1:K:209:GLU:HA    | 1:K:212:ASN:HD22  | 1.63                     | 0.62              |
| 2:M:101:ILE:HD13  | 2:M:107:LEU:HD22  | 1.79                     | 0.62              |
| 2:M:204:GLN:O     | 2:M:209:ARG:HD3   | 1.98                     | 0.62              |
| 2:M:660:ALA:HB1   | 2:M:667:ALA:O     | 2.00                     | 0.62              |
| 3:N:1213:ARG:HH11 | 3:N:1213:ARG:CG   | 2.11                     | 0.62              |
| 3:N:244:GLU:CG    | 3:N:245:LEU:H     | 2.12                     | 0.62              |
| 5:P:353:GLU:HA    | 5:P:356:LYS:CG    | 2.30                     | 0.62              |
| 5:P:80:PRO:HA     | 5:P:83:GLN:OE1    | 2.00                     | 0.62              |
| 5:P:93:LEU:O      | 5:P:93:LEU:HG     | 1.99                     | 0.62              |
| 1:B:76:VAL:O      | 1:B:80:LEU:HG     | 1.99                     | 0.62              |
| 2:C:1051:GLU:HG3  | 2:C:1052:MET:H    | 1.62                     | 0.62              |
| 2:C:267:TYR:CE1   | 2:C:464:LEU:HD12  | 2.34                     | 0.62              |
| 2:C:607:ASP:HB3   | 2:C:610:ARG:NH1   | 2.14                     | 0.62              |
| 3:D:1269:LYS:HE2  | 3:D:1269:LYS:H    | 1.63                     | 0.62              |
| 3:D:157:GLU:O     | 3:D:161:LEU:HG    | 1.97                     | 0.62              |
| 3:D:510:GLU:CD    | 3:D:510:GLU:H     | 2.02                     | 0.62              |
| 3:D:794:GLN:HE22  | 3:D:905:PRO:HG2   | 1.64                     | 0.62              |
| 3:D:841:TYR:HB2   | 3:D:864:VAL:CG1   | 2.29                     | 0.62              |
| 1:K:208:LEU:HG    | 1:K:209:GLU:N     | 2.14                     | 0.62              |
| 1:K:226:SER:O     | 1:K:228:PRO:HD3   | 1.99                     | 0.62              |
| 1:K:64:GLU:OE2    | 1:K:76:VAL:HG13   | 2.00                     | 0.62              |
| 1:L:48:ILE:C      | 1:L:148:VAL:HG12  | 2.20                     | 0.62              |
| 2:M:1059:ASP:OD2  | 2:M:1062:GLY:HA3  | 1.98                     | 0.62              |
| 2:M:1098:ASP:HB2  | 3:N:17:LYS:HE2    | 1.81                     | 0.62              |
| 2:M:781:LYS:HA    | 2:M:781:LYS:CE    | 2.28                     | 0.62              |
| 2:M:806:LEU:O     | 2:M:821:GLU:HB2   | 2.00                     | 0.62              |
| 2:M:549:PHE:CE2   | 2:M:886:LEU:HB2   | 2.33                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:984:GLU:O     | 3:N:946:GLY:HA3   | 2.00                     | 0.62              |
| 3:N:1031:ASN:ND2  | 3:N:1034:GLN:HG3  | 2.15                     | 0.62              |
| 3:N:1118:ILE:HD13 | 3:N:1190:SER:HB2  | 1.81                     | 0.62              |
| 3:N:1206:GLY:O    | 3:N:1215:VAL:HG12 | 1.99                     | 0.62              |
| 3:N:1342:GLU:N    | 3:N:1342:GLU:CD   | 2.52                     | 0.62              |
| 2:M:1085:PHE:CD2  | 3:N:1468:LEU:HA   | 2.34                     | 0.62              |
| 3:N:999:THR:O     | 3:N:1003:VAL:HG23 | 1.99                     | 0.62              |
| 1:A:1:MET:H1      | 1:A:6:LEU:HD13    | 1.63                     | 0.62              |
| 2:C:1100:GLN:HG3  | 2:C:1102:LEU:CD2  | 2.28                     | 0.62              |
| 2:C:191:PHE:HD2   | 2:C:195:LEU:HD11  | 1.64                     | 0.62              |
| 2:C:479:VAL:H     | 2:C:506:ASN:HB3   | 1.64                     | 0.62              |
| 3:D:1147:ARG:HB2  | 3:D:1166:LEU:HD12 | 1.81                     | 0.62              |
| 3:D:1217:ILE:HD12 | 3:D:1217:ILE:N    | 2.01                     | 0.62              |
| 3:D:269:PHE:CD1   | 3:D:283:PHE:HB2   | 2.33                     | 0.62              |
| 3:D:701:LEU:CD2   | 3:D:715:ALA:HB2   | 2.29                     | 0.62              |
| 3:D:1498:ALA:HB2  | 4:E:87:LYS:HZ3    | 1.63                     | 0.62              |
| 1:L:219:ARG:HG2   | 1:L:219:ARG:NH1   | 2.12                     | 0.62              |
| 2:M:170:PRO:CD    | 2:M:263:ASP:HB3   | 2.29                     | 0.62              |
| 2:M:773:LEU:CD1   | 2:M:777:ILE:HD11  | 2.28                     | 0.62              |
| 3:N:1121:PRO:HD2  | 3:N:1346:ARG:HH21 | 1.65                     | 0.62              |
| 3:N:139:GLY:HA3   | 3:N:147:VAL:HG23  | 1.79                     | 0.62              |
| 3:N:613:ARG:O     | 3:N:1441:GLN:HG3  | 2.00                     | 0.62              |
| 5:P:349:LEU:HA    | 5:P:352:GLU:OE2   | 1.99                     | 0.62              |
| 3:D:1246:VAL:HG11 | 3:D:1249:ALA:O    | 2.00                     | 0.62              |
| 3:D:1286:THR:HG22 | 3:D:1288:GLU:OE1  | 1.99                     | 0.62              |
| 3:D:272:LEU:HD12  | 3:D:282:TYR:CE1   | 2.33                     | 0.62              |
| 3:D:366:LYS:HE2   | 3:D:369:ALA:HB2   | 1.82                     | 0.62              |
| 3:D:984:THR:HG22  | 3:D:987:GLU:CG    | 2.30                     | 0.62              |
| 5:F:417:LYS:HB2   | 5:F:418:LEU:HD12  | 1.82                     | 0.62              |
| 1:L:26:GLU:HB2    | 1:L:27:PRO:HA     | 1.81                     | 0.62              |
| 1:L:57:TYR:CD1    | 1:L:163:ASN:HB2   | 2.34                     | 0.62              |
| 3:N:1379:VAL:C    | 3:N:1420:LEU:HD22 | 2.20                     | 0.62              |
| 3:N:658:LEU:O     | 3:N:661:MET:HB2   | 2.00                     | 0.62              |
| 3:N:954:ALA:HB3   | 3:N:1062:ARG:HD2  | 1.81                     | 0.62              |
| 5:P:152:ASP:N     | 5:P:153:PRO:CD    | 2.62                     | 0.62              |
| 1:B:47:SER:C      | 1:B:48:ILE:HD12   | 2.20                     | 0.62              |
| 1:B:64:GLU:HA     | 1:B:75:VAL:HG11   | 1.80                     | 0.62              |
| 3:D:1048:PRO:O    | 3:D:1079:LYS:NZ   | 2.32                     | 0.62              |
| 3:D:264:LEU:HB3   | 3:D:316:GLN:NE2   | 2.15                     | 0.62              |
| 3:D:551:ASN:O     | 3:D:554:LEU:HB3   | 1.99                     | 0.62              |
| 3:D:654:LYS:O     | 3:D:657:LEU:HB3   | 2.00                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1104:GLU:HA   | 3:D:7:LYS:HZ3     | 1.62                     | 0.62              |
| 4:E:61:GLU:CD     | 4:E:61:GLU:N      | 2.52                     | 0.62              |
| 1:L:68:ILE:HG13   | 1:L:71:VAL:O      | 2.00                     | 0.62              |
| 2:M:343:GLN:HG2   | 2:M:385:PHE:HB2   | 1.82                     | 0.62              |
| 2:M:672:VAL:HG23  | 2:M:673:LEU:N     | 2.13                     | 0.62              |
| 2:M:726:ILE:HG13  | 2:M:728:HIS:CB    | 2.29                     | 0.62              |
| 3:N:207:PHE:HB3   | 5:P:97:GLU:OE1    | 1.99                     | 0.62              |
| 3:N:27:GLU:HB2    | 3:N:28:LYS:HE2    | 1.81                     | 0.62              |
| 3:N:634:GLY:HA3   | 3:N:637:LEU:HG    | 1.82                     | 0.62              |
| 3:N:673:ALA:O     | 3:N:676:MET:HB3   | 2.00                     | 0.62              |
| 3:N:985:ASP:O     | 3:N:988:ARG:HB3   | 1.98                     | 0.62              |
| 3:N:989:TYR:O     | 3:N:992:ILE:HB    | 2.00                     | 0.62              |
| 5:P:305:GLU:O     | 5:P:308:LEU:HG    | 1.99                     | 0.62              |
| 2:C:555:ALA:O     | 2:C:558:ALA:HB3   | 1.99                     | 0.62              |
| 2:C:56:GLU:O      | 2:C:64:LEU:HD23   | 1.99                     | 0.62              |
| 2:C:672:VAL:CG2   | 2:C:673:LEU:N     | 2.63                     | 0.62              |
| 3:D:1381:VAL:HG12 | 3:D:1391:GLU:O    | 2.00                     | 0.62              |
| 3:D:1465:ASN:OD1  | 3:D:1470:ARG:HD3  | 2.00                     | 0.62              |
| 3:D:349:PRO:HB3   | 5:F:97:GLU:HG2    | 1.81                     | 0.62              |
| 3:D:657:LEU:HG    | 3:D:661:MET:HE2   | 1.80                     | 0.62              |
| 3:D:79:GLU:CG     | 3:D:80:VAL:H      | 2.11                     | 0.62              |
| 5:F:321:ILE:HG13  | 5:F:332:PHE:HE1   | 1.63                     | 0.62              |
| 1:L:153:ALA:HB2   | 1:L:168:ASP:N     | 2.14                     | 0.62              |
| 2:M:1037:VAL:HG12 | 2:M:1041:GLU:CD   | 2.19                     | 0.62              |
| 2:M:218:VAL:O     | 2:M:218:VAL:HG22  | 2.00                     | 0.62              |
| 2:M:522:VAL:HG12  | 2:M:523:ILE:N     | 2.15                     | 0.62              |
| 2:M:958:THR:HG23  | 2:M:961:GLU:HB3   | 1.80                     | 0.62              |
| 3:N:156:GLU:H     | 3:N:156:GLU:CD    | 2.04                     | 0.62              |
| 3:N:470:LEU:HB2   | 3:N:503:LEU:CD2   | 2.30                     | 0.62              |
| 3:N:865:THR:HA    | 3:N:873:LEU:O     | 2.00                     | 0.62              |
| 5:P:385:GLU:HA    | 5:P:388:ALA:HB3   | 1.80                     | 0.62              |
| 3:D:561:GLY:HA3   | 5:F:132:ARG:HD3   | 1.82                     | 0.62              |
| 5:F:132:ARG:NH2   | 5:F:184:ARG:HH12  | 1.96                     | 0.62              |
| 5:F:409:LYS:HD2   | 5:F:410:TYR:H     | 1.64                     | 0.62              |
| 1:K:178:ALA:HB2   | 2:M:864:GLY:N     | 2.15                     | 0.62              |
| 1:L:201:THR:HG21  | 1:L:207:PRO:HA    | 1.80                     | 0.62              |
| 2:M:205:GLU:CA    | 2:M:209:ARG:HH11  | 2.11                     | 0.62              |
| 3:N:1368:ILE:O    | 3:N:1372:VAL:HG23 | 1.99                     | 0.62              |
| 3:N:1462:LEU:HD23 | 3:N:1473:PRO:HD2  | 1.81                     | 0.62              |
| 3:N:249:TYR:HB3   | 3:N:307:ALA:CB    | 2.27                     | 0.62              |
| 3:N:479:GLU:O     | 3:N:481:MET:N     | 2.32                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:801:GLY:CA    | 3:N:830:ALA:HB3  | 2.30                     | 0.62              |
| 1:B:185:ARG:HB3   | 1:B:190:THR:HG23 | 1.80                     | 0.61              |
| 1:B:209:GLU:HA    | 1:B:212:ASN:ND2  | 2.14                     | 0.61              |
| 1:B:213:GLN:O     | 1:B:216:GLU:HB3  | 2.00                     | 0.61              |
| 2:C:672:VAL:HG23  | 2:C:868:ASP:HB2  | 1.81                     | 0.61              |
| 2:C:728:HIS:NE2   | 2:C:730:SER:HB3  | 2.15                     | 0.61              |
| 3:D:1086:LEU:HD12 | 3:D:1238:MET:SD  | 2.40                     | 0.61              |
| 3:D:136:ASP:CB    | 3:D:137:PRO:CD   | 2.78                     | 0.61              |
| 3:D:1486:VAL:HG22 | 4:E:75:PHE:CB    | 2.30                     | 0.61              |
| 3:D:937:TYR:H     | 3:D:937:TYR:HD1  | 1.46                     | 0.61              |
| 5:F:101:GLU:HG3   | 5:F:105:LYS:HE3  | 1.82                     | 0.61              |
| 5:F:223:ALA:HB2   | 5:F:242:TRP:HB2  | 1.82                     | 0.61              |
| 1:L:20:TYR:C      | 1:L:207:PRO:HG2  | 2.20                     | 0.61              |
| 2:M:328:LEU:HG    | 2:M:433:THR:CB   | 2.30                     | 0.61              |
| 2:M:606:VAL:HG22  | 2:M:645:VAL:HG13 | 1.81                     | 0.61              |
| 2:M:759:THR:HB    | 2:M:785:VAL:CG1  | 2.29                     | 0.61              |
| 3:N:1333:HIS:O    | 3:N:1336:LEU:HB3 | 2.00                     | 0.61              |
| 4:O:71:GLY:C      | 4:O:73:LEU:H     | 2.03                     | 0.61              |
| 5:P:102:LEU:HG    | 5:P:187:LEU:HD22 | 1.81                     | 0.61              |
| 5:P:382:THR:CG2   | 5:P:394:ARG:HB2  | 2.30                     | 0.61              |
| 1:B:215:VAL:HG23  | 1:B:216:GLU:N    | 2.15                     | 0.61              |
| 3:D:45:PHE:O      | 3:D:47:GLU:N     | 2.33                     | 0.61              |
| 3:D:915:VAL:O     | 3:D:918:ALA:HB3  | 2.00                     | 0.61              |
| 5:F:367:MET:HB3   | 5:F:371:LEU:HG   | 1.83                     | 0.61              |
| 1:L:90:LEU:HD12   | 1:L:119:ASP:HA   | 1.81                     | 0.61              |
| 2:M:18:LEU:HG     | 2:M:590:ASP:OD1  | 2.01                     | 0.61              |
| 2:M:230:ARG:HH21  | 2:M:237:ARG:HH22 | 0.77                     | 0.61              |
| 3:N:1468:LEU:HD23 | 3:N:1469:GLY:N   | 2.15                     | 0.61              |
| 3:N:553:ARG:NH1   | 5:P:211:ASP:HA   | 2.12                     | 0.61              |
| 5:P:353:GLU:HA    | 5:P:356:LYS:CD   | 2.29                     | 0.61              |
| 1:A:111:ALA:C     | 1:A:113:ASP:H    | 2.01                     | 0.61              |
| 1:A:206:THR:HG22  | 1:A:208:LEU:N    | 2.15                     | 0.61              |
| 2:C:373:VAL:HG12  | 2:C:374:ASN:N    | 2.15                     | 0.61              |
| 2:C:571:LEU:HD22  | 2:C:701:THR:N    | 2.15                     | 0.61              |
| 3:D:1183:ILE:HG13 | 3:D:1184:GLN:H   | 1.64                     | 0.61              |
| 3:D:1314:LYS:HB2  | 3:D:1317:ASP:OD2 | 1.99                     | 0.61              |
| 3:D:1424:VAL:HG23 | 3:D:1425:THR:N   | 2.14                     | 0.61              |
| 3:D:367:ILE:HD11  | 3:D:379:ALA:HA   | 1.82                     | 0.61              |
| 3:D:858:VAL:HG12  | 3:D:859:ASP:N    | 2.15                     | 0.61              |
| 4:E:87:LYS:HE3    | 4:E:91:ARG:NH2   | 2.16                     | 0.61              |
| 5:F:361:LEU:HG    | 5:F:362:SER:N    | 2.15                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:417:LYS:C    | 5:F:419:ARG:H    | 2.03                     | 0.61              |
| 1:K:110:LYS:CB   | 1:K:112:ARG:HG2  | 2.26                     | 0.61              |
| 2:M:182:VAL:HG22 | 2:M:220:GLY:O    | 1.99                     | 0.61              |
| 2:M:436:GLY:HA2  | 2:M:539:VAL:HA   | 1.81                     | 0.61              |
| 3:N:223:LEU:O    | 3:N:224:ARG:HD2  | 2.00                     | 0.61              |
| 3:N:417:PRO:HB3  | 3:N:430:ASP:CA   | 2.25                     | 0.61              |
| 3:N:479:GLU:C    | 3:N:481:MET:N    | 2.51                     | 0.61              |
| 2:M:1030:GLN:CG  | 3:N:626:SER:HB2  | 2.30                     | 0.61              |
| 3:N:350:HIS:HB3  | 5:P:232:ARG:NH1  | 2.14                     | 0.61              |
| 5:P:223:ALA:HB2  | 5:P:242:TRP:HB2  | 1.83                     | 0.61              |
| 2:C:101:ILE:CG2  | 2:C:107:LEU:HD23 | 2.30                     | 0.61              |
| 2:C:162:ILE:CD1  | 2:C:172:ILE:HD12 | 2.30                     | 0.61              |
| 2:C:631:SER:HB2  | 2:C:637:LEU:HD21 | 1.83                     | 0.61              |
| 2:C:6:PHE:HB3    | 2:C:908:GLY:HA2  | 1.81                     | 0.61              |
| 3:D:252:ARG:HG3  | 3:D:300:LYS:CA   | 2.29                     | 0.61              |
| 3:D:642:CYS:SG   | 3:D:716:PHE:HB2  | 2.40                     | 0.61              |
| 3:D:972:LEU:CD2  | 3:D:972:LEU:N    | 2.63                     | 0.61              |
| 5:F:288:TYR:HB3  | 5:F:301:ALA:CA   | 2.30                     | 0.61              |
| 5:F:74:LYS:O     | 5:F:77:THR:HB    | 2.00                     | 0.61              |
| 5:F:79:ASP:O     | 5:F:79:ASP:OD1   | 2.17                     | 0.61              |
| 1:K:101:LEU:HD13 | 1:K:113:ASP:O    | 2.01                     | 0.61              |
| 1:L:143:ARG:C    | 1:L:143:ARG:HD3  | 2.20                     | 0.61              |
| 2:M:687:ALA:HB1  | 2:M:850:ALA:HB2  | 1.81                     | 0.61              |
| 2:M:926:PHE:CD1  | 2:M:929:ARG:HG3  | 2.35                     | 0.61              |
| 3:N:206:ARG:NE   | 3:N:392:SER:HB2  | 2.15                     | 0.61              |
| 3:N:18:ILE:CG2   | 3:N:518:PRO:HG3  | 2.30                     | 0.61              |
| 3:N:633:VAL:O    | 3:N:635:PRO:HD3  | 1.99                     | 0.61              |
| 1:B:85:LEU:HD12  | 1:B:86:VAL:H     | 1.65                     | 0.61              |
| 2:C:317:VAL:N    | 2:C:318:PRO:CD   | 2.62                     | 0.61              |
| 2:C:138:SER:HB2  | 2:C:333:ILE:HD11 | 1.81                     | 0.61              |
| 2:C:431:HIS:CE1  | 2:C:433:THR:H    | 2.18                     | 0.61              |
| 3:D:133:ILE:O    | 3:D:152:LEU:HD12 | 2.00                     | 0.61              |
| 3:D:288:MET:HE2  | 3:D:307:ALA:HB2  | 1.81                     | 0.61              |
| 3:D:544:TYR:O    | 3:D:547:LEU:HB3  | 2.00                     | 0.61              |
| 5:F:267:THR:O    | 5:F:271:LEU:HG   | 1.99                     | 0.61              |
| 1:K:185:ARG:HA   | 1:K:190:THR:HA   | 1.82                     | 0.61              |
| 1:K:195:LEU:HD12 | 1:K:196:THR:N    | 2.14                     | 0.61              |
| 1:K:25:LEU:HD11  | 1:L:224:TYR:HB3  | 1.83                     | 0.61              |
| 2:M:1092:LEU:O   | 2:M:1095:LEU:HB2 | 2.00                     | 0.61              |
| 2:M:112:GLU:O    | 2:M:113:VAL:HG13 | 2.01                     | 0.61              |
| 2:M:493:ARG:HB2  | 2:M:494:TYR:CE1  | 2.35                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:676:ILE:CG2   | 2:M:988:VAL:HG13  | 2.31                     | 0.61              |
| 3:N:1032:PRO:HB2  | 3:N:1033:GLN:NE2  | 2.15                     | 0.61              |
| 3:N:567:ILE:HG22  | 3:N:571:LYS:CE    | 2.23                     | 0.61              |
| 2:M:1056:LYS:NZ   | 3:N:749:VAL:H     | 1.97                     | 0.61              |
| 3:N:811:GLU:HB2   | 3:N:816:HIS:CE1   | 2.35                     | 0.61              |
| 5:P:84:TYR:C      | 5:P:86:HIS:H      | 2.02                     | 0.61              |
| 1:B:101:LEU:HD22  | 1:B:114:PHE:CD1   | 2.35                     | 0.61              |
| 1:B:48:ILE:HG22   | 1:B:173:PRO:HD2   | 1.83                     | 0.61              |
| 2:C:676:ILE:O     | 2:C:676:ILE:HG12  | 1.99                     | 0.61              |
| 3:D:119:SER:C     | 3:D:121:THR:H     | 2.04                     | 0.61              |
| 3:D:1277:ILE:HG22 | 3:D:1278:ASP:N    | 2.08                     | 0.61              |
| 3:D:1368:ILE:O    | 3:D:1372:VAL:HG23 | 2.00                     | 0.61              |
| 3:D:204:LEU:HD12  | 3:D:205:TYR:N     | 2.15                     | 0.61              |
| 3:D:358:GLY:HA2   | 3:D:385:VAL:CB    | 2.29                     | 0.61              |
| 3:D:167:GLU:O     | 3:D:394:LEU:HD12  | 2.01                     | 0.61              |
| 3:D:661:MET:CE    | 3:D:677:LEU:HD11  | 2.30                     | 0.61              |
| 5:F:382:THR:HG22  | 5:F:394:ARG:CB    | 2.30                     | 0.61              |
| 2:M:200:LEU:HB2   | 2:M:202:TYR:CD2   | 2.35                     | 0.61              |
| 3:N:142:LEU:HD13  | 3:N:144:GLY:H     | 1.65                     | 0.61              |
| 3:N:1468:LEU:C    | 3:N:1468:LEU:HD23 | 2.19                     | 0.61              |
| 3:N:525:ARG:O     | 3:N:525:ARG:HG3   | 1.99                     | 0.61              |
| 3:N:820:GLU:HG3   | 3:N:836:VAL:CG1   | 2.31                     | 0.61              |
| 2:C:1058:ASP:HB3  | 2:C:1082:PRO:HB3  | 1.83                     | 0.61              |
| 2:C:263:ASP:HB2   | 2:C:264:PRO:CD    | 2.31                     | 0.61              |
| 2:C:352:ALA:O     | 2:C:355:VAL:HG12  | 2.00                     | 0.61              |
| 2:C:776:SER:HB3   | 2:C:780:GLU:CD    | 2.21                     | 0.61              |
| 3:D:953:ASP:OD2   | 3:D:1019:PRO:HG2  | 1.99                     | 0.61              |
| 3:D:257:GLY:HA2   | 3:D:274:ARG:CA    | 2.22                     | 0.61              |
| 3:D:406:ASP:CB    | 3:D:424:GLY:N     | 2.63                     | 0.61              |
| 3:D:806:PHE:CD2   | 3:D:809:PRO:HB2   | 2.34                     | 0.61              |
| 5:F:153:PRO:HG2   | 5:F:154:LYS:HG3   | 1.81                     | 0.61              |
| 1:L:179:PHE:CD1   | 1:L:195:LEU:HD11  | 2.36                     | 0.61              |
| 1:L:89:PHE:CD2    | 1:L:94:LEU:HB2    | 2.35                     | 0.61              |
| 2:M:89:THR:OG1    | 2:M:130:ASN:N     | 2.34                     | 0.61              |
| 2:M:944:LEU:HD21  | 2:M:963:LEU:CD2   | 2.30                     | 0.61              |
| 3:N:1015:TYR:N    | 3:N:1016:PRO:HD3  | 2.15                     | 0.61              |
| 3:N:225:LEU:HB3   | 3:N:226:PRO:CD    | 2.31                     | 0.61              |
| 3:N:483:HIS:H     | 3:N:483:HIS:HD1   | 1.47                     | 0.61              |
| 3:N:89:ARG:NH1    | 3:N:89:ARG:HG2    | 2.14                     | 0.61              |
| 5:P:372:ARG:HG3   | 5:P:378:GLY:O     | 2.00                     | 0.61              |
| 1:A:35:THR:O      | 1:A:39:PRO:HG2    | 2.00                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:143:ARG:HD3   | 1:B:143:ARG:C     | 2.21                     | 0.61              |
| 1:B:23:PHE:CD1    | 1:B:23:PHE:N      | 2.68                     | 0.61              |
| 2:C:334:ARG:NH1   | 2:C:418:LEU:HD11  | 2.15                     | 0.61              |
| 2:C:504:GLU:HG3   | 2:C:507:ARG:CD    | 2.30                     | 0.61              |
| 2:C:575:GLN:H     | 2:C:667:ALA:HB1   | 1.64                     | 0.61              |
| 2:C:549:PHE:CE2   | 2:C:886:LEU:HB2   | 2.36                     | 0.61              |
| 2:C:926:PHE:CD1   | 2:C:929:ARG:HG3   | 2.36                     | 0.61              |
| 3:D:1305:LEU:HD23 | 3:D:1305:LEU:N    | 2.15                     | 0.61              |
| 3:D:154:THR:HG22  | 3:D:157:GLU:OE2   | 2.01                     | 0.61              |
| 2:C:676:ILE:HD11  | 3:D:949:ILE:HB    | 1.83                     | 0.61              |
| 4:E:48:MET:O      | 4:E:54:LEU:HA     | 2.00                     | 0.61              |
| 2:M:1049:LEU:HD11 | 2:M:1053:LEU:HD11 | 1.83                     | 0.61              |
| 2:M:1085:PHE:CE2  | 3:N:1468:LEU:HA   | 2.34                     | 0.61              |
| 2:M:239:PHE:CZ    | 2:M:246:ASP:HB3   | 2.36                     | 0.61              |
| 2:M:649:VAL:HA    | 2:M:650:ARG:NH2   | 2.14                     | 0.61              |
| 3:N:1033:GLN:HA   | 3:N:1036:ARG:NH1  | 2.15                     | 0.61              |
| 3:N:1112:CYS:SG   | 3:N:1114:THR:HG22 | 2.41                     | 0.61              |
| 3:N:284:LEU:HB3   | 3:N:288:MET:HB3   | 1.81                     | 0.61              |
| 3:N:93:ILE:HB     | 3:N:517:VAL:HB    | 1.82                     | 0.61              |
| 5:P:113:ILE:HD13  | 5:P:128:ARG:HB3   | 1.83                     | 0.61              |
| 3:N:349:PRO:CB    | 5:P:232:ARG:HH22  | 2.12                     | 0.61              |
| 5:P:367:MET:HB2   | 5:P:371:LEU:CD1   | 2.30                     | 0.61              |
| 1:B:114:PHE:O     | 1:B:116:PRO:HD3   | 2.01                     | 0.61              |
| 2:C:187:ASN:O     | 2:C:188:LYS:HG2   | 2.00                     | 0.61              |
| 2:C:230:ARG:CG    | 2:C:233:GLU:HG3   | 2.22                     | 0.61              |
| 2:C:937:ASP:HB3   | 2:C:940:GLU:HG3   | 1.81                     | 0.61              |
| 2:C:946:ARG:HH11  | 2:C:984:GLU:HB2   | 1.66                     | 0.61              |
| 3:D:1033:GLN:H    | 3:D:1033:GLN:CD   | 2.04                     | 0.61              |
| 3:D:1122:LEU:HG   | 3:D:1184:GLN:O    | 2.01                     | 0.61              |
| 3:D:881:LEU:HD21  | 3:D:941:PHE:HZ    | 1.65                     | 0.61              |
| 1:L:241:GLU:H     | 1:L:242:PRO:CD    | 2.10                     | 0.61              |
| 2:M:1067:TYR:CE1  | 2:M:1071:ILE:HD11 | 2.35                     | 0.61              |
| 2:M:685:GLU:HB3   | 3:N:740:PHE:CD1   | 2.36                     | 0.61              |
| 2:M:910:LYS:N     | 2:M:913:GLU:OE1   | 2.34                     | 0.61              |
| 3:N:1094:LEU:CD1  | 3:N:1098:LEU:HD11 | 2.29                     | 0.61              |
| 3:N:1126:ASP:OD1  | 3:N:1129:THR:HA   | 2.01                     | 0.61              |
| 3:N:112:ILE:O     | 3:N:115:LEU:HB3   | 2.00                     | 0.61              |
| 3:N:1305:LEU:N    | 3:N:1305:LEU:HD23 | 2.15                     | 0.61              |
| 3:N:1367:HIS:HA   | 3:N:1370:ILE:HD12 | 1.83                     | 0.61              |
| 3:N:322:VAL:HB    | 3:N:335:LEU:HD21  | 1.83                     | 0.61              |
| 3:N:809:PRO:HA    | 3:N:810:GLU:OE2   | 2.01                     | 0.61              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:881:LEU:HD21 | 3:N:941:PHE:CZ   | 2.35                     | 0.61              |
| 1:B:219:ARG:HG2  | 1:B:219:ARG:HH11 | 1.65                     | 0.61              |
| 2:C:1015:LEU:O   | 2:C:1018:GLN:NE2 | 2.34                     | 0.61              |
| 2:C:178:PRO:O    | 2:C:220:GLY:CA   | 2.32                     | 0.61              |
| 2:C:303:PHE:CD1  | 2:C:303:PHE:N    | 2.69                     | 0.61              |
| 2:C:666:LEU:HD12 | 2:C:667:ALA:N    | 2.16                     | 0.61              |
| 2:C:813:VAL:CG1  | 2:C:815:LEU:HG   | 2.31                     | 0.61              |
| 3:D:100:ALA:HA   | 3:D:513:ILE:HD12 | 1.83                     | 0.61              |
| 3:D:1137:ARG:O   | 3:D:1141:GLU:HG3 | 2.01                     | 0.61              |
| 3:D:833:GLU:N    | 3:D:833:GLU:CD   | 2.54                     | 0.61              |
| 3:D:852:ALA:HB1  | 3:D:857:ILE:HD11 | 1.83                     | 0.61              |
| 5:F:144:ILE:O    | 5:F:144:ILE:HG13 | 2.01                     | 0.61              |
| 5:F:380:GLU:N    | 5:F:385:GLU:OE2  | 2.34                     | 0.61              |
| 1:K:73:GLU:CD    | 1:K:131:THR:H    | 2.04                     | 0.61              |
| 1:L:101:LEU:HD22 | 1:L:114:PHE:CD1  | 2.35                     | 0.61              |
| 1:L:233:VAL:HG12 | 1:L:235:ALA:H    | 1.66                     | 0.61              |
| 2:M:261:ILE:CG2  | 2:M:262:ALA:N    | 2.64                     | 0.61              |
| 2:M:689:VAL:O    | 2:M:690:ILE:HD13 | 2.00                     | 0.61              |
| 3:N:121:THR:CG2  | 3:N:122:GLU:H    | 2.01                     | 0.61              |
| 3:N:1400:VAL:HA  | 3:N:1408:ILE:CD1 | 2.30                     | 0.61              |
| 5:P:271:LEU:N    | 5:P:271:LEU:HD23 | 2.16                     | 0.61              |
| 2:C:683:ASN:H    | 2:C:683:ASN:ND2  | 1.98                     | 0.60              |
| 5:F:370:LYS:HG3  | 5:F:371:LEU:N    | 2.14                     | 0.60              |
| 2:M:224:GLU:HB3  | 2:M:227:PHE:CG   | 2.36                     | 0.60              |
| 2:M:285:LEU:HD11 | 2:M:288:ARG:C    | 2.21                     | 0.60              |
| 2:M:400:PRO:HB3  | 2:M:591:SER:HB2  | 1.82                     | 0.60              |
| 2:M:486:MET:SD   | 2:M:491:GLU:N    | 2.74                     | 0.60              |
| 2:M:923:GLU:O    | 2:M:927:GLY:N    | 2.34                     | 0.60              |
| 3:N:1008:PHE:HZ  | 3:N:1032:PRO:HA  | 1.64                     | 0.60              |
| 3:N:141:ILE:CB   | 3:N:450:TYR:HD2  | 2.13                     | 0.60              |
| 3:N:230:TRP:NE1  | 3:N:233:LYS:HG3  | 2.16                     | 0.60              |
| 3:N:280:ALA:HB1  | 3:N:282:TYR:OH   | 2.01                     | 0.60              |
| 3:N:287:GLY:O    | 3:N:311:LEU:HD22 | 2.01                     | 0.60              |
| 3:N:401:TYR:CE2  | 3:N:429:SER:HB2  | 2.36                     | 0.60              |
| 3:N:408:GLU:CB   | 3:N:422:ALA:HB2  | 2.28                     | 0.60              |
| 3:N:501:ALA:O    | 3:N:505:SER:HB2  | 2.01                     | 0.60              |
| 3:N:660:LYS:HG3  | 3:N:694:VAL:HG22 | 1.83                     | 0.60              |
| 3:N:828:LYS:N    | 3:N:828:LYS:CD   | 2.64                     | 0.60              |
| 3:N:807:ALA:HA   | 3:N:833:GLU:HB2  | 1.83                     | 0.60              |
| 5:P:86:HIS:C     | 5:P:88:ILE:H     | 2.03                     | 0.60              |
| 2:C:233:GLU:HB2  | 2:C:237:ARG:NH2  | 2.15                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:250:ARG:CB    | 2:C:253:ALA:HB2   | 2.31                     | 0.60              |
| 2:C:483:VAL:HG22  | 2:C:484:VAL:N     | 2.16                     | 0.60              |
| 2:C:496:ILE:HA    | 2:C:531:PHE:O     | 2.01                     | 0.60              |
| 2:C:896:PHE:C     | 2:C:898:GLY:H     | 2.04                     | 0.60              |
| 3:D:15:PRO:O      | 3:D:19:ARG:HG3    | 2.01                     | 0.60              |
| 3:D:241:ILE:HG12  | 3:D:312:ARG:HG3   | 1.82                     | 0.60              |
| 3:D:355:VAL:HG21  | 3:D:367:ILE:HG23  | 1.81                     | 0.60              |
| 3:D:401:TYR:O     | 3:D:444:VAL:HG22  | 2.02                     | 0.60              |
| 3:D:433:GLY:CA    | 3:D:449:SER:H     | 2.04                     | 0.60              |
| 2:M:1035:MET:HA   | 2:M:1038:TRP:CE3  | 2.35                     | 0.60              |
| 2:M:1060:ILE:O    | 2:M:1063:ARG:HG2  | 2.00                     | 0.60              |
| 2:M:157:ARG:NH1   | 2:M:314:THR:HA    | 2.16                     | 0.60              |
| 2:M:36:PRO:HG2    | 2:M:38:LYS:HB3    | 1.84                     | 0.60              |
| 3:N:1122:LEU:O    | 3:N:1134:LEU:HD12 | 2.00                     | 0.60              |
| 3:N:131:LYS:HE3   | 3:N:565:ILE:HA    | 1.83                     | 0.60              |
| 3:N:1321:ALA:O    | 3:N:1339:LYS:HG3  | 2.01                     | 0.60              |
| 3:N:139:GLY:HA2   | 3:N:452:ILE:HG22  | 1.81                     | 0.60              |
| 3:N:348:GLN:HB2   | 3:N:351:MET:SD    | 2.41                     | 0.60              |
| 3:N:356:PRO:HB3   | 3:N:440:VAL:CB    | 2.28                     | 0.60              |
| 3:N:44:LEU:O      | 3:N:525:ARG:NH2   | 2.33                     | 0.60              |
| 3:N:924:MET:O     | 3:N:927:THR:HB    | 2.01                     | 0.60              |
| 3:N:968:ASP:HA    | 3:N:971:LEU:HD12  | 1.82                     | 0.60              |
| 1:B:218:LEU:O     | 1:B:221:HIS:HB2   | 2.01                     | 0.60              |
| 2:C:1021:LEU:HD21 | 5:F:332:PHE:O     | 2.01                     | 0.60              |
| 2:C:1049:LEU:O    | 2:C:1052:MET:HB3  | 2.01                     | 0.60              |
| 2:C:13:ILE:HD13   | 2:C:13:ILE:H      | 1.66                     | 0.60              |
| 2:C:654:LEU:HD12  | 2:C:655:LEU:N     | 2.13                     | 0.60              |
| 3:D:408:GLU:CG    | 3:D:422:ALA:HB2   | 2.31                     | 0.60              |
| 3:D:593:ASN:HB3   | 3:D:594:PRO:HD3   | 1.84                     | 0.60              |
| 3:D:951:ILE:HD11  | 3:D:1062:ARG:CG   | 2.26                     | 0.60              |
| 5:F:340:SER:N     | 5:F:343:ASP:OD2   | 2.34                     | 0.60              |
| 5:F:367:MET:HA    | 5:F:370:LYS:HG2   | 1.83                     | 0.60              |
| 1:L:38:ASN:ND2    | 2:M:979:THR:HA    | 2.17                     | 0.60              |
| 2:M:326:ASP:HA    | 2:M:331:ARG:HD2   | 1.82                     | 0.60              |
| 2:M:355:VAL:CA    | 2:M:358:ARG:HG3   | 2.30                     | 0.60              |
| 3:N:104:PHE:N     | 3:N:104:PHE:CD1   | 2.68                     | 0.60              |
| 3:N:1302:GLU:HG2  | 3:N:1303:TYR:H    | 1.67                     | 0.60              |
| 3:N:126:VAL:O     | 3:N:132:TYR:CD1   | 2.53                     | 0.60              |
| 3:N:1406:ARG:HD3  | 3:N:1412:LYS:HZ1  | 1.66                     | 0.60              |
| 3:N:1450:ALA:O    | 3:N:1454:GLY:N    | 2.34                     | 0.60              |
| 3:N:729:HIS:HE1   | 3:N:935:LYS:NZ    | 1.99                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:566:ILE:HG21  | 5:P:192:LEU:HD22  | 1.83                     | 0.60              |
| 5:P:245:GLN:HA    | 5:P:245:GLN:HE21  | 1.66                     | 0.60              |
| 1:B:13:VAL:CG2    | 1:B:14:ARG:H      | 2.15                     | 0.60              |
| 1:A:35:THR:N      | 1:B:42:ARG:NH1    | 2.48                     | 0.60              |
| 2:C:1021:LEU:HD23 | 5:F:334:PRO:HB3   | 1.83                     | 0.60              |
| 2:C:352:ALA:CA    | 2:C:355:VAL:HG12  | 2.27                     | 0.60              |
| 2:C:36:PRO:HG2    | 2:C:38:LYS:HG2    | 1.83                     | 0.60              |
| 3:D:1498:ALA:HA   | 3:D:1501:GLU:HB2  | 1.82                     | 0.60              |
| 3:D:274:ARG:HH21  | 3:D:279:VAL:HG13  | 1.65                     | 0.60              |
| 3:D:248:PRO:CA    | 3:D:308:LYS:HZ3   | 2.09                     | 0.60              |
| 3:D:323:GLU:HB2   | 3:D:334:THR:OG1   | 2.00                     | 0.60              |
| 3:D:634:GLY:HA3   | 3:D:637:LEU:HG    | 1.83                     | 0.60              |
| 3:D:713:ILE:O     | 3:D:714:GLN:HG3   | 2.02                     | 0.60              |
| 3:D:729:HIS:O     | 3:D:732:VAL:HG22  | 2.01                     | 0.60              |
| 3:D:82:LYS:O      | 3:D:85:VAL:HG12   | 2.01                     | 0.60              |
| 1:L:48:ILE:HG22   | 1:L:173:PRO:HD2   | 1.82                     | 0.60              |
| 1:L:211:LEU:O     | 1:L:215:VAL:HG13  | 2.01                     | 0.60              |
| 2:M:722:ILE:HG13  | 2:M:722:ILE:O     | 2.01                     | 0.60              |
| 3:N:106:LYS:HA    | 3:N:106:LYS:CE    | 2.25                     | 0.60              |
| 3:N:1097:LYS:HB2  | 3:N:1098:LEU:HD12 | 1.84                     | 0.60              |
| 3:N:1341:PRO:HA   | 3:N:1344:VAL:HG12 | 1.83                     | 0.60              |
| 3:N:1466:VAL:O    | 3:N:1468:LEU:N    | 2.34                     | 0.60              |
| 3:N:1099:VAL:CG1  | 10:N:1528:NE6:H14 | 2.29                     | 0.60              |
| 3:N:243:ALA:HB3   | 3:N:311:LEU:CD1   | 2.30                     | 0.60              |
| 3:N:274:ARG:NE    | 3:N:279:VAL:HG11  | 2.17                     | 0.60              |
| 3:N:355:VAL:HG13  | 3:N:356:PRO:HD2   | 1.83                     | 0.60              |
| 3:N:367:ILE:HB    | 3:N:377:VAL:HG11  | 1.82                     | 0.60              |
| 3:N:351:MET:HA    | 3:N:370:ALA:HB2   | 1.84                     | 0.60              |
| 3:N:59:ALA:HB3    | 3:N:76:CYS:CB     | 2.31                     | 0.60              |
| 1:A:34:VAL:O      | 1:A:36:LEU:N      | 2.34                     | 0.60              |
| 2:C:202:TYR:HB2   | 2:C:207:LEU:HD11  | 1.84                     | 0.60              |
| 2:C:873:PRO:O     | 2:C:876:VAL:HG23  | 2.01                     | 0.60              |
| 3:D:1117:TYR:CD1  | 3:D:1118:ILE:N    | 2.69                     | 0.60              |
| 3:D:1152:GLU:HG2  | 3:D:1153:VAL:H    | 1.66                     | 0.60              |
| 3:D:241:ILE:CD1   | 3:D:310:LEU:HD22  | 2.30                     | 0.60              |
| 3:D:322:VAL:CG2   | 3:D:333:LEU:HD22  | 2.31                     | 0.60              |
| 3:D:341:GLU:OE1   | 3:D:343:LYS:HE3   | 2.02                     | 0.60              |
| 3:D:210:ARG:HB2   | 3:D:389:GLU:HB2   | 1.82                     | 0.60              |
| 2:M:305:PRO:HA    | 2:M:308:ARG:HG2   | 1.83                     | 0.60              |
| 2:M:42:VAL:HG13   | 2:M:43:GLY:N      | 2.17                     | 0.60              |
| 3:N:1107:VAL:HG11 | 3:N:1217:ILE:HA   | 1.84                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:212:ARG:HD3   | 3:N:342:PRO:HB3  | 1.83                     | 0.60              |
| 3:N:362:GLU:H     | 3:N:365:ASP:CB   | 2.15                     | 0.60              |
| 3:N:671:LYS:HE2   | 3:N:675:ARG:HD3  | 1.82                     | 0.60              |
| 5:P:200:LYS:HA    | 5:P:209:PHE:HE1  | 1.66                     | 0.60              |
| 1:A:108:GLU:HG2   | 1:A:109:VAL:N    | 2.15                     | 0.60              |
| 1:A:55:SER:HB2    | 1:A:165:ILE:O    | 2.02                     | 0.60              |
| 1:B:63:HIS:CD2    | 1:B:65:PHE:HB2   | 2.36                     | 0.60              |
| 2:C:34:VAL:N      | 2:C:35:PRO:CD    | 2.64                     | 0.60              |
| 2:C:71:TYR:HD2    | 2:C:71:TYR:N     | 1.97                     | 0.60              |
| 3:D:1442:ASN:HD21 | 3:D:1445:HIS:HB2 | 1.66                     | 0.60              |
| 5:F:86:HIS:C      | 5:F:88:ILE:H     | 2.05                     | 0.60              |
| 1:K:100:LEU:HB3   | 1:K:115:LEU:CD1  | 2.28                     | 0.60              |
| 1:L:87:VAL:HG12   | 1:L:122:ILE:HA   | 1.84                     | 0.60              |
| 1:L:75:VAL:O      | 1:L:79:ILE:HG13  | 2.02                     | 0.60              |
| 2:M:41:ASN:HB2    | 2:M:46:ALA:HA    | 1.82                     | 0.60              |
| 2:M:61:LYS:O      | 2:M:103:LYS:HB2  | 2.01                     | 0.60              |
| 3:N:1019:PRO:O    | 3:N:1023:MET:HG3 | 2.00                     | 0.60              |
| 3:N:227:LEU:HD12  | 3:N:331:VAL:HG22 | 1.82                     | 0.60              |
| 5:P:367:MET:O     | 5:P:370:LYS:HG2  | 2.02                     | 0.60              |
| 1:A:138:LEU:HD12  | 1:A:139:ASN:N    | 2.14                     | 0.60              |
| 2:C:1112:PHE:O    | 2:C:1113:GLU:HG2 | 2.01                     | 0.60              |
| 2:C:415:PRO:O     | 2:C:419:THR:N    | 2.32                     | 0.60              |
| 2:C:790:LEU:HD12  | 2:C:791:ARG:N    | 2.15                     | 0.60              |
| 3:D:1341:PRO:O    | 3:D:1343:ALA:N   | 2.35                     | 0.60              |
| 3:D:136:ASP:HB3   | 3:D:137:PRO:CD   | 2.28                     | 0.60              |
| 3:D:1405:GLU:CD   | 3:D:1406:ARG:H   | 2.04                     | 0.60              |
| 3:D:172:PRO:HB2   | 3:D:175:VAL:HG21 | 1.83                     | 0.60              |
| 3:D:658:LEU:O     | 3:D:661:MET:HB2  | 2.02                     | 0.60              |
| 3:D:673:ALA:CA    | 3:D:676:MET:HB3  | 2.32                     | 0.60              |
| 3:D:828:LYS:H     | 3:D:828:LYS:HD3  | 1.67                     | 0.60              |
| 3:D:1485:GLN:O    | 4:E:75:PHE:HA    | 2.02                     | 0.60              |
| 5:F:101:GLU:CG    | 5:F:105:LYS:HE3  | 2.32                     | 0.60              |
| 5:F:308:LEU:HD23  | 5:F:308:LEU:H    | 1.66                     | 0.60              |
| 1:K:110:LYS:HB3   | 1:K:125:PRO:O    | 2.02                     | 0.60              |
| 1:L:123:MET:HE2   | 1:L:204:SER:HA   | 1.83                     | 0.60              |
| 2:M:276:LYS:HB3   | 2:M:280:LYS:HZ2  | 1.65                     | 0.60              |
| 2:M:974:LEU:HB2   | 2:M:983:ILE:HD12 | 1.83                     | 0.60              |
| 3:N:1165:TYR:CE2  | 3:N:1206:GLY:HA2 | 2.36                     | 0.60              |
| 3:N:462:GLN:HG2   | 3:N:466:LYS:HE3  | 1.83                     | 0.60              |
| 3:N:675:ARG:O     | 3:N:678:GLU:HG2  | 2.02                     | 0.60              |
| 3:N:769:LEU:O     | 3:N:778:LEU:N    | 2.27                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:151:LEU:C     | 5:P:153:PRO:HD2   | 2.22                     | 0.60              |
| 5:P:253:ASP:CB    | 5:P:259:ARG:HH12  | 2.15                     | 0.60              |
| 5:P:282:LEU:C     | 5:P:284:ARG:H     | 2.05                     | 0.60              |
| 1:A:20:TYR:HD1    | 1:A:199:ILE:O     | 1.85                     | 0.60              |
| 1:A:224:TYR:HD2   | 1:A:224:TYR:N     | 2.00                     | 0.60              |
| 1:B:80:LEU:HB3    | 3:D:844:ALA:HB2   | 1.83                     | 0.60              |
| 2:C:353:ARG:O     | 2:C:357:GLU:HG3   | 2.02                     | 0.60              |
| 2:C:100:LEU:CD2   | 2:C:367:LEU:HD23  | 2.30                     | 0.60              |
| 2:C:56:GLU:HB2    | 2:C:64:LEU:HD23   | 1.84                     | 0.60              |
| 2:C:573:ARG:HB2   | 2:C:670:GLN:NE2   | 2.16                     | 0.60              |
| 2:C:649:VAL:HG22  | 2:C:650:ARG:HH21  | 1.67                     | 0.60              |
| 2:C:760:SER:O     | 2:C:786:LYS:N     | 2.34                     | 0.60              |
| 3:D:1038:LEU:HD23 | 3:D:1061:PHE:HB2  | 1.84                     | 0.60              |
| 3:D:1264:GLU:OE2  | 3:D:1424:VAL:HG22 | 2.02                     | 0.60              |
| 3:D:142:LEU:HD13  | 3:D:144:GLY:H     | 1.66                     | 0.60              |
| 3:D:376:GLU:O     | 3:D:378:ILE:HG13  | 2.01                     | 0.60              |
| 3:D:834:THR:HA    | 3:D:838:ARG:HD2   | 1.84                     | 0.60              |
| 5:F:263:HIS:HA    | 5:F:266:GLU:CD    | 2.21                     | 0.60              |
| 5:F:367:MET:O     | 5:F:370:LYS:HG2   | 2.02                     | 0.60              |
| 1:K:1:MET:H1      | 1:K:6:LEU:HD22    | 1.67                     | 0.60              |
| 1:L:58:ILE:HB     | 1:L:61:VAL:CG1    | 2.31                     | 0.60              |
| 2:M:542:VAL:CG2   | 2:M:543:ASN:H     | 2.07                     | 0.60              |
| 2:M:550:LEU:HD12  | 2:M:550:LEU:O     | 2.01                     | 0.60              |
| 3:N:1162:GLU:O    | 3:N:1162:GLU:HG3  | 2.02                     | 0.60              |
| 3:N:170:PRO:C     | 3:N:171:LEU:HD23  | 2.21                     | 0.60              |
| 2:M:774:LEU:HD23  | 5:P:418:LEU:CD2   | 2.31                     | 0.60              |
| 1:A:231:ALA:N     | 1:B:13:VAL:O      | 2.30                     | 0.60              |
| 2:C:66:LEU:HA     | 2:C:99:GLN:O      | 2.02                     | 0.60              |
| 2:C:939:ARG:NH1   | 2:C:942:GLU:OE2   | 2.34                     | 0.60              |
| 3:D:1000:THR:HG23 | 3:D:1041:LEU:HD23 | 1.83                     | 0.60              |
| 3:D:1041:LEU:CD1  | 3:D:1058:ARG:HA   | 2.32                     | 0.60              |
| 3:D:1066:THR:N    | 3:D:1069:GLU:HB2  | 2.16                     | 0.60              |
| 3:D:1286:THR:CG2  | 3:D:1289:LYS:H    | 2.15                     | 0.60              |
| 3:D:302:GLN:N     | 3:D:303:PRO:HD2   | 2.16                     | 0.60              |
| 3:D:167:GLU:O     | 3:D:394:LEU:HA    | 2.02                     | 0.60              |
| 3:D:400:VAL:HG23  | 3:D:443:VAL:HG11  | 1.81                     | 0.60              |
| 3:D:699:VAL:HG12  | 3:D:717:GLN:CG    | 2.31                     | 0.60              |
| 5:F:175:HIS:O     | 5:F:178:ARG:HB2   | 2.02                     | 0.60              |
| 3:D:65:ARG:HB3    | 5:F:375:LEU:O     | 2.02                     | 0.60              |
| 2:M:369:PRO:O     | 2:M:372:LEU:HD21  | 2.01                     | 0.60              |
| 3:N:1208:ASP:CG   | 3:N:1211:MET:HG2  | 2.22                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:1268:PRO:O   | 3:N:1271:LYS:HB2  | 2.02                     | 0.60              |
| 3:N:617:ASN:HB3  | 3:N:619:LEU:HG    | 1.84                     | 0.60              |
| 3:N:867:ARG:HA   | 3:N:871:LYS:O     | 2.01                     | 0.60              |
| 5:P:169:GLU:H    | 5:P:169:GLU:CD    | 2.04                     | 0.60              |
| 2:C:1048:THR:O   | 2:C:1051:GLU:HG3  | 2.02                     | 0.60              |
| 2:C:185:LYS:HE2  | 2:C:190:LYS:NZ    | 2.17                     | 0.60              |
| 2:C:504:GLU:HG3  | 2:C:507:ARG:HD2   | 1.84                     | 0.60              |
| 2:C:474:VAL:HG12 | 2:C:530:GLU:C     | 2.22                     | 0.60              |
| 2:C:683:ASN:HD22 | 2:C:683:ASN:H     | 1.50                     | 0.60              |
| 2:C:710:ILE:HD13 | 2:C:790:LEU:HB2   | 1.83                     | 0.60              |
| 3:D:1045:MET:HG3 | 3:D:1073:SER:HA   | 1.83                     | 0.60              |
| 3:D:297:ILE:HG23 | 3:D:298:VAL:N     | 2.17                     | 0.60              |
| 3:D:295:GLY:C    | 3:D:302:GLN:HB3   | 2.21                     | 0.60              |
| 3:D:463:GLN:HB3  | 3:D:467:GLU:OE2   | 2.01                     | 0.60              |
| 3:D:911:LEU:O    | 3:D:914:LEU:HB3   | 2.02                     | 0.60              |
| 5:F:234:LYS:CE   | 5:F:236:SER:HB3   | 2.32                     | 0.60              |
| 1:K:152:PRO:CG   | 1:K:155:LYS:HB2   | 2.29                     | 0.60              |
| 2:M:228:ALA:O    | 2:M:229:MET:HG3   | 2.02                     | 0.60              |
| 2:M:71:TYR:CD2   | 2:M:71:TYR:N      | 2.68                     | 0.60              |
| 3:N:1107:VAL:CG1 | 3:N:1217:ILE:HA   | 2.32                     | 0.60              |
| 3:N:1403:LEU:HB3 | 3:N:1408:ILE:HD12 | 1.83                     | 0.60              |
| 3:N:252:ARG:HG3  | 3:N:300:LYS:CA    | 2.32                     | 0.60              |
| 3:N:860:LEU:O    | 3:N:876:SER:HB2   | 2.01                     | 0.60              |
| 3:N:939:PHE:O    | 3:N:940:THR:C     | 2.40                     | 0.60              |
| 5:P:298:GLY:O    | 5:P:303:ARG:NH1   | 2.35                     | 0.60              |
| 5:P:367:MET:CE   | 5:P:371:LEU:HD21  | 2.32                     | 0.60              |
| 2:C:93:PRO:HA    | 2:C:117:HIS:CB    | 2.31                     | 0.59              |
| 2:C:12:VAL:HG23  | 2:C:13:ILE:HD12   | 1.84                     | 0.59              |
| 2:C:18:LEU:C     | 2:C:20:GLU:H      | 2.04                     | 0.59              |
| 2:C:233:GLU:CD   | 2:C:234:ALA:N     | 2.53                     | 0.59              |
| 2:C:691:SER:CB   | 2:C:868:ASP:HA    | 2.31                     | 0.59              |
| 3:D:1117:TYR:C   | 3:D:1193:THR:HG21 | 2.22                     | 0.59              |
| 3:D:1286:THR:HB  | 3:D:1289:LYS:H    | 1.66                     | 0.59              |
| 3:D:259:VAL:HG21 | 3:D:292:VAL:O     | 2.02                     | 0.59              |
| 3:D:408:GLU:OE2  | 3:D:422:ALA:HB2   | 2.01                     | 0.59              |
| 3:D:483:HIS:HB2  | 3:D:484:PRO:CD    | 2.27                     | 0.59              |
| 3:D:799:LYS:HB3  | 3:D:800:LYS:HE2   | 1.83                     | 0.59              |
| 3:D:811:GLU:HB3  | 3:D:815:ALA:HB3   | 1.84                     | 0.59              |
| 3:D:901:GLN:HB3  | 3:D:904:VAL:CG2   | 2.32                     | 0.59              |
| 1:K:100:LEU:CD2  | 1:K:101:LEU:H     | 2.12                     | 0.59              |
| 1:K:211:LEU:O    | 1:K:214:ALA:HB3   | 2.02                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:36:LEU:O     | 1:K:39:PRO:HD2    | 2.02                     | 0.59              |
| 1:K:86:VAL:CG1   | 1:K:123:MET:HB2   | 2.32                     | 0.59              |
| 1:L:209:GLU:O    | 1:L:213:GLN:HG3   | 2.02                     | 0.59              |
| 1:L:5:LYS:C      | 1:L:7:LYS:N       | 2.55                     | 0.59              |
| 1:L:99:LEU:HB3   | 1:L:114:PHE:CE2   | 2.37                     | 0.59              |
| 2:M:1090:LYS:HE2 | 2:M:1112:PHE:CZ   | 2.37                     | 0.59              |
| 3:N:1173:LEU:O   | 3:N:1176:LYS:HB3  | 2.02                     | 0.59              |
| 3:N:774:SER:HB3  | 3:N:1362:LYS:O    | 2.02                     | 0.59              |
| 3:N:1478:SER:O   | 3:N:1482:ARG:HG3  | 2.01                     | 0.59              |
| 3:N:167:GLU:O    | 3:N:394:LEU:HA    | 2.02                     | 0.59              |
| 3:N:32:ILE:HG12  | 3:N:39:PRO:HA     | 1.84                     | 0.59              |
| 3:N:433:GLY:HA3  | 3:N:448:GLU:HA    | 1.84                     | 0.59              |
| 1:A:76:VAL:HA    | 1:A:79:ILE:CD1    | 2.27                     | 0.59              |
| 2:C:154:ARG:HG2  | 2:C:156:GLY:H     | 1.67                     | 0.59              |
| 2:C:182:VAL:HG21 | 2:C:194:VAL:CG2   | 2.32                     | 0.59              |
| 2:C:492:ASP:CA   | 2:C:518:LYS:HB3   | 2.31                     | 0.59              |
| 2:C:700:TYR:HB2  | 2:C:833:LEU:HD22  | 1.83                     | 0.59              |
| 2:C:966:LEU:HD21 | 2:C:986:PRO:CG    | 2.32                     | 0.59              |
| 3:D:41:ARG:HH21  | 3:D:48:ARG:CZ     | 2.14                     | 0.59              |
| 3:D:527:MET:HA   | 3:D:537:THR:HG23  | 1.83                     | 0.59              |
| 5:F:353:GLU:HA   | 5:F:356:LYS:CG    | 2.31                     | 0.59              |
| 1:K:11:PHE:HB2   | 1:L:224:TYR:O     | 2.02                     | 0.59              |
| 2:M:401:LEU:O    | 2:M:405:ARG:N     | 2.34                     | 0.59              |
| 2:M:504:GLU:O    | 2:M:507:ARG:HD2   | 2.02                     | 0.59              |
| 2:M:498:GLN:HA   | 2:M:533:ASP:OD2   | 2.01                     | 0.59              |
| 2:M:595:LEU:O    | 2:M:654:LEU:HD12  | 2.01                     | 0.59              |
| 3:N:658:LEU:CA   | 3:N:661:MET:HE3   | 2.31                     | 0.59              |
| 3:N:661:MET:O    | 3:N:664:LYS:O     | 2.21                     | 0.59              |
| 3:N:84:ILE:O     | 3:N:87:ARG:HG2    | 2.02                     | 0.59              |
| 1:A:35:THR:C     | 1:A:36:LEU:HD12   | 2.22                     | 0.59              |
| 1:B:38:ASN:O     | 1:B:42:ARG:HG3    | 2.02                     | 0.59              |
| 2:C:1030:GLN:HG2 | 3:D:626:SER:HB2   | 1.83                     | 0.59              |
| 2:C:166:PRO:HG2  | 2:C:169:GLY:N     | 2.17                     | 0.59              |
| 2:C:321:GLU:CD   | 2:C:321:GLU:H     | 2.06                     | 0.59              |
| 2:C:585:GLU:HB2  | 2:C:665:PHE:CE2   | 2.36                     | 0.59              |
| 3:D:1031:ASN:OD1 | 3:D:1034:GLN:HG3  | 2.01                     | 0.59              |
| 3:D:103:TRP:CZ2  | 3:D:604:THR:HG23  | 2.37                     | 0.59              |
| 3:D:1121:PRO:HG2 | 3:D:1135:ARG:HH11 | 1.66                     | 0.59              |
| 3:D:1170:ASP:O   | 3:D:1173:LEU:HB3  | 2.02                     | 0.59              |
| 3:D:1405:GLU:CG  | 3:D:1406:ARG:H    | 2.14                     | 0.59              |
| 3:D:400:VAL:HG22 | 3:D:402:PRO:HD3   | 1.84                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:639:LEU:O     | 3:D:639:LEU:HD12 | 2.01                     | 0.59              |
| 3:D:654:LYS:CB    | 3:D:655:PRO:HD3  | 2.32                     | 0.59              |
| 1:K:218:LEU:O     | 1:K:221:HIS:HB2  | 2.02                     | 0.59              |
| 2:M:333:ILE:HG22  | 2:M:465:GLY:O    | 2.02                     | 0.59              |
| 2:M:474:VAL:HG12  | 2:M:530:GLU:C    | 2.22                     | 0.59              |
| 2:M:504:GLU:HG3   | 2:M:507:ARG:HB2  | 1.84                     | 0.59              |
| 2:M:497:ALA:HA    | 2:M:515:ALA:HA   | 1.84                     | 0.59              |
| 2:M:713:ARG:HD2   | 2:M:720:GLU:OE2  | 2.01                     | 0.59              |
| 3:N:1273:VAL:HG23 | 3:N:1325:LEU:HB2 | 1.84                     | 0.59              |
| 3:N:1341:PRO:O    | 3:N:1344:VAL:N   | 2.35                     | 0.59              |
| 3:N:135:LEU:HD12  | 3:N:148:GLU:CB   | 2.33                     | 0.59              |
| 3:N:408:GLU:HB2   | 3:N:421:LEU:O    | 2.02                     | 0.59              |
| 3:N:960:LYS:HG2   | 3:N:964:LEU:CD1  | 2.32                     | 0.59              |
| 3:N:966:GLU:HA    | 3:N:969:ARG:NE   | 2.17                     | 0.59              |
| 3:N:968:ASP:O     | 3:N:971:LEU:HB2  | 2.03                     | 0.59              |
| 5:P:300:ASP:HB3   | 5:P:302:LYS:HZ2  | 1.67                     | 0.59              |
| 1:A:181:VAL:HG13  | 1:A:193:ASP:HB3  | 1.85                     | 0.59              |
| 1:A:78:ILE:O      | 1:A:82:LEU:HG    | 2.02                     | 0.59              |
| 1:B:59:GLU:HB2    | 1:B:139:ASN:HD22 | 1.67                     | 0.59              |
| 1:B:176:ARG:HB3   | 1:B:200:TRP:CD1  | 2.37                     | 0.59              |
| 2:C:166:PRO:HG3   | 2:C:263:ASP:HA   | 1.84                     | 0.59              |
| 2:C:17:PRO:HD2    | 2:C:20:GLU:OE1   | 2.01                     | 0.59              |
| 2:C:430:VAL:O     | 2:C:430:VAL:HG13 | 2.02                     | 0.59              |
| 2:C:807:ARG:C     | 2:C:809:GLY:N    | 2.52                     | 0.59              |
| 2:C:682:TYR:CE1   | 2:C:851:LYS:HD2  | 2.37                     | 0.59              |
| 2:C:930:LYS:C     | 2:C:932:GLU:H    | 2.04                     | 0.59              |
| 3:D:1066:THR:HG22 | 3:D:1068:LEU:H   | 1.67                     | 0.59              |
| 3:D:1048:PRO:HA   | 3:D:1079:LYS:HE3 | 1.83                     | 0.59              |
| 3:D:1288:GLU:O    | 3:D:1307:LYS:HD3 | 2.03                     | 0.59              |
| 3:D:1335:LEU:CD2  | 3:D:1344:VAL:HA  | 2.32                     | 0.59              |
| 3:D:433:GLY:C     | 3:D:434:ARG:HD2  | 2.23                     | 0.59              |
| 3:D:658:LEU:HD23  | 3:D:661:MET:CE   | 2.32                     | 0.59              |
| 3:D:921:ARG:HB3   | 3:D:921:ARG:NH1  | 2.17                     | 0.59              |
| 1:L:201:THR:CG2   | 1:L:207:PRO:HA   | 2.32                     | 0.59              |
| 2:M:164:PRO:HG3   | 2:M:170:PRO:HB2  | 1.83                     | 0.59              |
| 2:M:198:ARG:NH2   | 2:M:231:PRO:HD3  | 2.16                     | 0.59              |
| 2:M:226:VAL:HA    | 2:M:229:MET:SD   | 2.42                     | 0.59              |
| 2:M:617:ASP:OD2   | 2:M:619:ARG:HG3  | 2.03                     | 0.59              |
| 3:N:149:LYS:HE2   | 3:N:151:GLN:HG3  | 1.83                     | 0.59              |
| 3:N:362:GLU:H     | 3:N:365:ASP:HB2  | 1.66                     | 0.59              |
| 3:N:361:VAL:CG1   | 3:N:379:ALA:HB1  | 2.32                     | 0.59              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:140:ALA:N     | 3:N:450:TYR:CE2  | 2.70                     | 0.59              |
| 3:N:605:ASP:O     | 3:N:609:GLY:HA2  | 2.02                     | 0.59              |
| 3:N:984:THR:HG22  | 3:N:987:GLU:CB   | 2.33                     | 0.59              |
| 2:C:283:ILE:CG2   | 2:C:284:ARG:H    | 2.03                     | 0.59              |
| 2:C:571:LEU:HD13  | 2:C:699:PHE:O    | 2.02                     | 0.59              |
| 2:C:929:ARG:O     | 2:C:934:PHE:HB2  | 2.03                     | 0.59              |
| 3:D:1047:LYS:HD2  | 3:D:1051:GLU:CG  | 2.32                     | 0.59              |
| 3:D:163:TYR:O     | 3:D:447:VAL:HG11 | 2.02                     | 0.59              |
| 3:D:820:GLU:CG    | 3:D:836:VAL:HG11 | 2.26                     | 0.59              |
| 2:M:187:ASN:O     | 2:M:188:LYS:HG3  | 2.02                     | 0.59              |
| 2:M:261:ILE:C     | 2:M:288:ARG:HH21 | 2.06                     | 0.59              |
| 2:M:31:GLN:NE2    | 2:M:40:GLU:O     | 2.35                     | 0.59              |
| 2:M:688:ILE:HD11  | 2:M:847:GLY:HA3  | 1.84                     | 0.59              |
| 2:M:881:ASN:N     | 2:M:881:ASN:ND2  | 2.50                     | 0.59              |
| 3:N:1161:GLU:HG3  | 3:N:1164:ARG:CB  | 2.32                     | 0.59              |
| 3:N:387:LEU:CD1   | 3:N:387:LEU:H    | 2.16                     | 0.59              |
| 3:N:527:MET:SD    | 3:N:537:THR:HG21 | 2.42                     | 0.59              |
| 3:N:551:ASN:O     | 3:N:555:LYS:HG3  | 2.01                     | 0.59              |
| 2:C:140:ILE:HG23  | 2:C:410:ILE:HG21 | 1.84                     | 0.59              |
| 2:C:205:GLU:CA    | 2:C:209:ARG:HH11 | 2.16                     | 0.59              |
| 2:C:816:LYS:H     | 2:C:816:LYS:HD2  | 1.68                     | 0.59              |
| 3:D:826:PRO:HB2   | 3:D:829:VAL:HG13 | 1.82                     | 0.59              |
| 3:D:995:LEU:HG    | 3:D:996:TRP:N    | 2.17                     | 0.59              |
| 4:E:87:LYS:HG2    | 4:E:88:GLU:N     | 2.17                     | 0.59              |
| 5:F:167:PRO:HD2   | 5:F:170:HIS:HD2  | 1.66                     | 0.59              |
| 5:F:204:GLY:O     | 5:F:206:GLY:N    | 2.36                     | 0.59              |
| 5:F:330:GLY:HA2   | 5:F:333:ILE:HD12 | 1.82                     | 0.59              |
| 5:F:77:THR:O      | 5:F:77:THR:HG23  | 2.03                     | 0.59              |
| 1:K:14:ARG:CD     | 1:L:233:VAL:HA   | 2.32                     | 0.59              |
| 1:K:206:THR:HB    | 1:K:209:GLU:CD   | 2.22                     | 0.59              |
| 1:L:98:THR:HA     | 1:L:142:VAL:O    | 2.02                     | 0.59              |
| 2:M:385:PHE:HD1   | 2:M:389:SER:HB2  | 1.68                     | 0.59              |
| 2:M:776:SER:HB3   | 5:P:379:ARG:NH2  | 2.14                     | 0.59              |
| 2:M:841:ASN:ND2   | 2:M:845:ASN:HB3  | 2.18                     | 0.59              |
| 1:K:176:ARG:CZ    | 2:M:865:THR:CG2  | 2.81                     | 0.59              |
| 3:N:1147:ARG:O    | 3:N:1166:LEU:HG  | 2.03                     | 0.59              |
| 3:N:1398:TRP:O    | 3:N:1402:ALA:N   | 2.35                     | 0.59              |
| 3:N:297:ILE:CG2   | 3:N:298:VAL:H    | 2.13                     | 0.59              |
| 3:N:204:LEU:O     | 3:N:393:ILE:HG23 | 2.03                     | 0.59              |
| 3:D:1107:VAL:CG1  | 3:D:1217:ILE:HA  | 2.32                     | 0.59              |
| 3:D:1495:ILE:HG13 | 4:E:84:ARG:HH12  | 1.68                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:122:ILE:CG2  | 1:K:124:ASN:H     | 2.08                     | 0.59              |
| 1:L:56:VAL:HG12  | 1:L:57:TYR:N      | 2.17                     | 0.59              |
| 2:M:1068:GLU:O   | 2:M:1072:LYS:HG2  | 2.03                     | 0.59              |
| 2:M:405:ARG:NH2  | 2:M:409:ARG:CZ    | 2.65                     | 0.59              |
| 3:N:334:THR:C    | 3:N:335:LEU:HD12  | 2.23                     | 0.59              |
| 5:P:184:ARG:O    | 5:P:188:ILE:HG13  | 2.02                     | 0.59              |
| 5:P:370:LYS:HA   | 5:P:374:GLY:HA3   | 1.83                     | 0.59              |
| 2:C:560:MET:HB3  | 2:C:564:MET:CE    | 2.33                     | 0.59              |
| 3:D:165:LYS:O    | 3:D:396:VAL:HA    | 2.02                     | 0.59              |
| 3:D:355:VAL:HG13 | 3:D:356:PRO:HD2   | 1.85                     | 0.59              |
| 3:D:565:ILE:HG23 | 3:D:566:ILE:H     | 1.67                     | 0.59              |
| 3:D:807:ALA:HA   | 3:D:833:GLU:CG    | 2.32                     | 0.59              |
| 2:M:101:ILE:CG2  | 2:M:102:HIS:H     | 2.14                     | 0.59              |
| 2:M:195:LEU:HB3  | 2:M:238:LEU:HD21  | 1.84                     | 0.59              |
| 2:M:310:LEU:O    | 2:M:314:THR:HG23  | 2.02                     | 0.59              |
| 2:M:355:VAL:HA   | 2:M:358:ARG:HE    | 1.67                     | 0.59              |
| 2:M:42:VAL:CG1   | 2:M:43:GLY:N      | 2.66                     | 0.59              |
| 2:M:463:GLU:H    | 2:M:463:GLU:CD    | 2.06                     | 0.59              |
| 2:M:69:LEU:HB3   | 2:M:97:ARG:HB2    | 1.85                     | 0.59              |
| 3:N:1434:TRP:CE3 | 3:N:1457:ASP:HB2  | 2.38                     | 0.59              |
| 3:N:475:LYS:O    | 3:N:478:LEU:HB3   | 2.03                     | 0.59              |
| 1:B:112:ARG:CB   | 1:B:112:ARG:HH11  | 2.16                     | 0.59              |
| 1:B:41:ARG:HG3   | 1:B:41:ARG:HH11   | 1.68                     | 0.59              |
| 2:C:1050:GLN:HG2 | 2:C:1079:PRO:HG2  | 1.83                     | 0.59              |
| 2:C:269:LEU:HD12 | 2:C:288:ARG:CB    | 2.31                     | 0.59              |
| 2:C:632:ASN:HB3  | 2:C:633:GLN:HE22  | 1.67                     | 0.59              |
| 3:D:1489:GLN:NE2 | 4:E:72:ARG:HA     | 2.17                     | 0.59              |
| 3:D:709:HIS:CD2  | 3:D:711:LEU:HB2   | 2.38                     | 0.59              |
| 3:D:881:LEU:O    | 3:D:885:ILE:HG13  | 2.02                     | 0.59              |
| 5:F:79:ASP:OD1   | 5:F:82:ARG:HB2    | 2.03                     | 0.59              |
| 1:L:76:VAL:O     | 1:L:79:ILE:HB     | 2.02                     | 0.59              |
| 2:M:198:ARG:HE   | 2:M:231:PRO:CD    | 2.15                     | 0.59              |
| 2:M:243:ARG:HG3  | 2:M:244:PRO:CA    | 2.24                     | 0.59              |
| 3:N:10:ILE:HG23  | 3:N:10:ILE:O      | 2.03                     | 0.59              |
| 3:N:1108:ARG:NE  | 3:N:1199:GLY:HA3  | 2.18                     | 0.59              |
| 3:N:1217:ILE:N   | 3:N:1217:ILE:HD12 | 2.05                     | 0.59              |
| 3:N:252:ARG:HG3  | 3:N:300:LYS:HA    | 1.84                     | 0.59              |
| 3:N:58:CYS:HB2   | 3:N:76:CYS:SG     | 2.42                     | 0.59              |
| 5:P:111:GLU:HG3  | 5:P:114:LYS:NZ    | 2.15                     | 0.59              |
| 5:P:111:GLU:O    | 5:P:114:LYS:HB2   | 2.03                     | 0.59              |
| 5:P:222:ARG:HG2  | 5:P:242:TRP:CZ3   | 2.37                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:386:VAL:HG23  | 5:P:387:GLY:H     | 1.67                     | 0.59              |
| 5:P:77:THR:O      | 5:P:79:ASP:N      | 2.36                     | 0.59              |
| 1:B:238:GLU:HB3   | 1:B:240:LYS:HZ2   | 1.68                     | 0.59              |
| 2:C:917:LEU:HD23  | 2:C:920:GLN:OE1   | 2.03                     | 0.59              |
| 3:D:1085:ALA:HA   | 3:D:1088:THR:CG2  | 2.32                     | 0.59              |
| 3:D:1422:MET:SD   | 3:D:1427:SER:HA   | 2.43                     | 0.59              |
| 3:D:1474:ALA:O    | 3:D:1477:GLY:N    | 2.36                     | 0.59              |
| 3:D:966:GLU:HA    | 3:D:969:ARG:CZ    | 2.33                     | 0.59              |
| 5:F:392:VAL:CG1   | 5:F:396:ARG:HD3   | 2.30                     | 0.59              |
| 1:K:188:GLN:CG    | 1:K:189:ARG:H     | 2.03                     | 0.59              |
| 2:M:1005:MET:HG2  | 3:N:629:SER:CB    | 2.31                     | 0.59              |
| 2:M:588:VAL:CG2   | 2:M:589:ARG:N     | 2.64                     | 0.59              |
| 2:M:712:ALA:O     | 2:M:820:ARG:HG3   | 2.03                     | 0.59              |
| 1:L:42:ARG:HH22   | 2:M:939:ARG:NH2   | 2.00                     | 0.59              |
| 3:N:121:THR:O     | 3:N:122:GLU:C     | 2.40                     | 0.59              |
| 3:N:554:LEU:O     | 3:N:555:LYS:C     | 2.41                     | 0.59              |
| 5:P:329:TYR:O     | 5:P:332:PHE:HD1   | 1.84                     | 0.59              |
| 1:B:235:ALA:CB    | 1:B:236:PRO:HD3   | 2.30                     | 0.58              |
| 2:C:421:GLU:O     | 2:C:421:GLU:HG2   | 2.02                     | 0.58              |
| 3:D:1403:LEU:HD23 | 3:D:1408:ILE:HD11 | 1.82                     | 0.58              |
| 3:D:274:ARG:NE    | 3:D:279:VAL:HG11  | 2.17                     | 0.58              |
| 3:D:248:PRO:CB    | 3:D:308:LYS:HZ1   | 2.16                     | 0.58              |
| 3:D:800:LYS:HZ1   | 3:D:826:PRO:HD3   | 1.68                     | 0.58              |
| 1:K:111:ALA:CA    | 1:K:129:ILE:HD11  | 2.31                     | 0.58              |
| 1:K:88:ARG:HD2    | 1:K:90:LEU:HD23   | 1.84                     | 0.58              |
| 2:M:185:LYS:CG    | 2:M:190:LYS:HD3   | 2.29                     | 0.58              |
| 2:M:352:ALA:CA    | 2:M:355:VAL:HG12  | 2.31                     | 0.58              |
| 2:M:582:GLY:O     | 2:M:584:GLU:HG2   | 2.03                     | 0.58              |
| 2:M:813:VAL:CG1   | 2:M:815:LEU:HG    | 2.33                     | 0.58              |
| 3:N:127:LEU:HD23  | 3:N:128:TYR:CA    | 2.32                     | 0.58              |
| 3:N:1376:MET:HA   | 3:N:1376:MET:HE2  | 1.84                     | 0.58              |
| 3:N:1491:THR:C    | 3:N:1493:LYS:H    | 2.06                     | 0.58              |
| 3:N:225:LEU:HD12  | 3:N:333:LEU:CD1   | 2.32                     | 0.58              |
| 4:O:33:HIS:HB2    | 4:O:37:ASN:OD1    | 2.02                     | 0.58              |
| 2:C:399:ASN:HB2   | 2:C:400:PRO:CD    | 2.33                     | 0.58              |
| 3:D:211:VAL:HG13  | 3:D:386:HIS:O     | 2.03                     | 0.58              |
| 3:D:525:ARG:N     | 3:D:526:PRO:CD    | 2.63                     | 0.58              |
| 4:E:28:GLN:O      | 4:E:32:ARG:HG3    | 2.03                     | 0.58              |
| 1:K:184:THR:HG23  | 1:K:192:LEU:HB2   | 1.85                     | 0.58              |
| 2:M:301:GLU:HA    | 2:M:304:LEU:CD2   | 2.26                     | 0.58              |
| 2:M:545:ASN:HB3   | 2:M:583:LEU:HD11  | 1.85                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:595:LEU:HD21  | 2:M:639:GLN:HE22  | 1.67                     | 0.58              |
| 2:M:815:LEU:HD11  | 2:M:821:GLU:HA    | 1.85                     | 0.58              |
| 3:N:1068:LEU:O    | 3:N:1072:ILE:HG13 | 2.04                     | 0.58              |
| 1:A:169:ALA:HB1   | 1:A:171:PHE:CE1   | 2.38                     | 0.58              |
| 1:B:44:LEU:O      | 1:B:174:VAL:HG21  | 2.03                     | 0.58              |
| 2:C:267:TYR:CB    | 2:C:272:ALA:HB2   | 2.16                     | 0.58              |
| 2:C:1:MET:CB      | 2:C:899:GLN:HA    | 2.33                     | 0.58              |
| 3:D:1384:PRO:HB3  | 3:D:1387:SER:O    | 2.04                     | 0.58              |
| 3:D:274:ARG:CB    | 3:D:279:VAL:HG21  | 2.17                     | 0.58              |
| 3:D:564:GLU:O     | 3:D:567:ILE:HB    | 2.03                     | 0.58              |
| 1:B:154:GLU:HG2   | 3:D:840:LYS:HE3   | 1.85                     | 0.58              |
| 3:D:972:LEU:N     | 3:D:972:LEU:HD22  | 2.18                     | 0.58              |
| 3:D:1498:ALA:HB3  | 4:E:84:ARG:NE     | 2.19                     | 0.58              |
| 5:F:172:ARG:HG3   | 5:F:173:TYR:N     | 2.17                     | 0.58              |
| 5:F:269:ASN:O     | 5:F:273:ARG:HG3   | 2.03                     | 0.58              |
| 5:F:303:ARG:O     | 5:F:304:VAL:C     | 2.40                     | 0.58              |
| 2:M:232:GLU:O     | 2:M:236:ILE:HG13  | 2.03                     | 0.58              |
| 2:M:689:VAL:CG2   | 2:M:870:ILE:HB    | 2.32                     | 0.58              |
| 2:M:774:LEU:HD23  | 5:P:418:LEU:HD23  | 1.84                     | 0.58              |
| 3:N:1035:ILE:O    | 3:N:1038:LEU:N    | 2.36                     | 0.58              |
| 3:N:167:GLU:HB3   | 3:N:169:TYR:CZ    | 2.38                     | 0.58              |
| 3:N:167:GLU:HB3   | 3:N:169:TYR:OH    | 2.02                     | 0.58              |
| 3:N:699:VAL:CG1   | 3:N:717:GLN:HG2   | 2.28                     | 0.58              |
| 3:N:917:GLN:O     | 3:N:921:ARG:HG2   | 2.03                     | 0.58              |
| 4:O:49:GLN:HA     | 4:O:53:GLY:O      | 2.03                     | 0.58              |
| 2:C:1054:THR:HG22 | 2:C:1082:PRO:HG3  | 1.86                     | 0.58              |
| 2:C:176:VAL:C     | 2:C:178:PRO:HD3   | 2.22                     | 0.58              |
| 2:C:198:ARG:HA    | 2:C:202:TYR:O     | 2.03                     | 0.58              |
| 2:C:615:TYR:O     | 2:C:618:GLY:N     | 2.37                     | 0.58              |
| 3:D:1364:HIS:CE1  | 3:D:1366:LYS:HG3  | 2.38                     | 0.58              |
| 3:D:241:ILE:HG13  | 3:D:312:ARG:CZ    | 2.33                     | 0.58              |
| 3:D:408:GLU:OE1   | 3:D:444:VAL:HG11  | 2.03                     | 0.58              |
| 2:C:874:LEU:HD13  | 3:D:783:ARG:HB3   | 1.86                     | 0.58              |
| 3:D:792:ILE:HG21  | 3:D:941:PHE:CD1   | 2.37                     | 0.58              |
| 3:D:887:ALA:CB    | 3:D:893:GLU:HA    | 2.33                     | 0.58              |
| 3:D:894:LYS:O     | 3:D:898:GLU:HG3   | 2.02                     | 0.58              |
| 5:F:147:LEU:O     | 5:F:148:LYS:HB2   | 2.02                     | 0.58              |
| 1:K:9:PRO:HG2     | 1:K:28:LEU:CD2    | 2.33                     | 0.58              |
| 1:K:74:ASP:O      | 1:K:75:VAL:C      | 2.42                     | 0.58              |
| 1:K:75:VAL:O      | 1:K:79:ILE:HG13   | 2.04                     | 0.58              |
| 1:L:52:ALA:HB1    | 1:L:170:VAL:H     | 1.67                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:1033:GLY:O    | 2:M:1037:VAL:HG23 | 2.03                     | 0.58              |
| 2:M:1072:LYS:HB2  | 2:M:1074:GLU:HG3  | 1.84                     | 0.58              |
| 2:M:385:PHE:O     | 2:M:389:SER:N     | 2.37                     | 0.58              |
| 2:M:79:PRO:HG2    | 2:M:82:GLU:HB2    | 1.84                     | 0.58              |
| 2:M:835:VAL:HA    | 2:M:849:VAL:CG1   | 2.34                     | 0.58              |
| 3:N:1117:TYR:CA   | 3:N:1193:THR:HG21 | 2.32                     | 0.58              |
| 3:N:1086:LEU:HD12 | 3:N:1238:MET:SD   | 2.44                     | 0.58              |
| 3:N:1398:TRP:HA   | 3:N:1401:GLU:HB2  | 1.84                     | 0.58              |
| 3:N:280:ALA:HB1   | 3:N:282:TYR:CE1   | 2.38                     | 0.58              |
| 3:N:799:LYS:H     | 3:N:829:VAL:CG1   | 2.16                     | 0.58              |
| 3:N:826:PRO:HD2   | 3:N:829:VAL:CG1   | 2.30                     | 0.58              |
| 4:O:61:GLU:CD     | 4:O:61:GLU:H      | 2.07                     | 0.58              |
| 2:C:122:THR:HG22  | 2:C:123:GLU:H     | 1.68                     | 0.58              |
| 2:C:204:GLN:NE2   | 2:C:225:SER:HB3   | 2.18                     | 0.58              |
| 2:C:18:LEU:C      | 2:C:20:GLU:N      | 2.54                     | 0.58              |
| 2:C:614:ARG:HE    | 2:C:618:GLY:HA2   | 1.68                     | 0.58              |
| 2:C:710:ILE:CG2   | 2:C:823:VAL:HB    | 2.32                     | 0.58              |
| 2:C:937:ASP:O     | 2:C:940:GLU:HB2   | 2.04                     | 0.58              |
| 3:D:252:ARG:HA    | 3:D:301:GLY:HA3   | 1.85                     | 0.58              |
| 3:D:241:ILE:HG12  | 3:D:312:ARG:CG    | 2.33                     | 0.58              |
| 5:F:113:ILE:HA    | 5:F:116:LEU:CD1   | 2.23                     | 0.58              |
| 5:F:223:ALA:HB2   | 5:F:242:TRP:CB    | 2.33                     | 0.58              |
| 5:F:321:ILE:HD11  | 5:F:329:TYR:N     | 2.18                     | 0.58              |
| 5:F:371:LEU:HA    | 5:F:375:LEU:CG    | 2.31                     | 0.58              |
| 1:K:107:LYS:HE2   | 1:K:108:GLU:O     | 2.04                     | 0.58              |
| 1:L:128:HIS:HE1   | 1:L:131:THR:HG23  | 1.69                     | 0.58              |
| 2:M:327:HIS:HB3   | 2:M:330:ASN:ND2   | 2.18                     | 0.58              |
| 2:M:44:ILE:HG23   | 2:M:344:PHE:CE1   | 2.28                     | 0.58              |
| 2:M:712:ALA:HB3   | 2:M:821:GLU:H     | 1.68                     | 0.58              |
| 2:M:906:PHE:HZ    | 3:N:1070:TYR:CD2  | 2.21                     | 0.58              |
| 3:N:796:ARG:NE    | 3:N:861:GLN:HB2   | 2.18                     | 0.58              |
| 5:P:167:PRO:HD2   | 5:P:170:HIS:HD2   | 1.67                     | 0.58              |
| 2:C:195:LEU:CD2   | 2:C:195:LEU:H     | 1.93                     | 0.58              |
| 2:C:467:ILE:HG22  | 2:C:468:ARG:N     | 2.18                     | 0.58              |
| 3:D:160:GLU:C     | 3:D:161:LEU:HD23  | 2.24                     | 0.58              |
| 3:D:298:VAL:HB    | 3:D:300:LYS:HE3   | 1.86                     | 0.58              |
| 3:D:490:ALA:O     | 3:D:493:ARG:HG2   | 2.03                     | 0.58              |
| 3:D:540:LEU:O     | 3:D:544:TYR:N     | 2.33                     | 0.58              |
| 3:D:542:ASP:HA    | 3:D:545:ARG:HG3   | 1.84                     | 0.58              |
| 3:D:591:VAL:HG12  | 3:D:599:PRO:HA    | 1.84                     | 0.58              |
| 3:D:800:LYS:CD    | 3:D:800:LYS:H     | 2.17                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:843:PHE:CD1   | 3:D:849:ALA:HA   | 2.39                     | 0.58              |
| 3:D:990:ASP:C     | 3:D:994:GLN:HE21 | 2.07                     | 0.58              |
| 4:E:84:ARG:O      | 4:E:87:LYS:HB3   | 2.04                     | 0.58              |
| 3:D:563:PRO:HG3   | 5:F:185:GLN:OE1  | 2.04                     | 0.58              |
| 5:F:189:GLU:CA    | 5:F:192:LEU:HG   | 2.26                     | 0.58              |
| 5:F:85:LEU:C      | 5:F:87:GLU:H     | 2.07                     | 0.58              |
| 1:K:122:ILE:HG22  | 1:K:123:MET:N    | 2.17                     | 0.58              |
| 1:L:151:VAL:HB    | 1:L:169:ALA:HB3  | 1.84                     | 0.58              |
| 1:L:23:PHE:N      | 1:L:23:PHE:CD1   | 2.71                     | 0.58              |
| 2:M:857:ASP:CB    | 2:M:978:ARG:HG2  | 2.34                     | 0.58              |
| 3:N:1472:ILE:HG22 | 3:N:1474:ALA:H   | 1.68                     | 0.58              |
| 2:M:1098:ASP:HB2  | 3:N:17:LYS:CE    | 2.33                     | 0.58              |
| 3:N:27:GLU:C      | 3:N:28:LYS:HD3   | 2.24                     | 0.58              |
| 3:N:221:ALA:O     | 3:N:334:THR:HG23 | 2.04                     | 0.58              |
| 3:N:100:ALA:HA    | 3:N:513:ILE:HD12 | 1.85                     | 0.58              |
| 3:N:661:MET:HB3   | 3:N:667:ALA:HB2  | 1.85                     | 0.58              |
| 5:P:157:GLU:H     | 5:P:157:GLU:CD   | 2.06                     | 0.58              |
| 5:P:214:GLN:O     | 5:P:217:ASN:HB2  | 2.04                     | 0.58              |
| 5:P:270:LYS:HE3   | 5:P:295:MET:SD   | 2.43                     | 0.58              |
| 3:N:536:ALA:C     | 5:P:317:LEU:HD21 | 2.24                     | 0.58              |
| 5:P:382:THR:HG23  | 5:P:397:ILE:HG21 | 1.85                     | 0.58              |
| 2:C:122:THR:HG22  | 2:C:123:GLU:N    | 2.17                     | 0.58              |
| 2:C:511:GLU:O     | 2:C:525:SER:HA   | 2.04                     | 0.58              |
| 2:C:572:ILE:CD1   | 2:C:701:THR:HB   | 2.33                     | 0.58              |
| 2:C:73:LEU:HB3    | 2:C:93:PRO:O     | 2.03                     | 0.58              |
| 3:D:152:LEU:HG    | 3:D:153:LEU:N    | 2.18                     | 0.58              |
| 3:D:438:ASP:O     | 3:D:439:LEU:HD23 | 2.03                     | 0.58              |
| 3:D:99:ALA:O      | 3:D:514:LEU:HB2  | 2.03                     | 0.58              |
| 4:E:84:ARG:O      | 4:E:88:GLU:HG2   | 2.04                     | 0.58              |
| 1:K:138:LEU:HD21  | 1:K:140:MET:HE3  | 1.86                     | 0.58              |
| 2:M:310:LEU:HD12  | 2:M:314:THR:HG23 | 1.86                     | 0.58              |
| 3:N:149:LYS:HG2   | 3:N:150:ARG:HG2  | 1.84                     | 0.58              |
| 3:N:187:LYS:HG3   | 3:N:198:ARG:HA   | 1.86                     | 0.58              |
| 3:N:469:ASP:OD1   | 3:N:471:GLU:HB2  | 2.03                     | 0.58              |
| 1:A:128:HIS:CE1   | 1:A:131:THR:HG23 | 2.39                     | 0.58              |
| 2:C:232:GLU:O     | 2:C:235:LEU:HB3  | 2.04                     | 0.58              |
| 2:C:293:PHE:CD1   | 2:C:294:GLU:HG3  | 2.39                     | 0.58              |
| 2:C:100:LEU:HD21  | 2:C:367:LEU:CD2  | 2.33                     | 0.58              |
| 2:C:636:ALA:O     | 2:C:637:LEU:HD23 | 2.04                     | 0.58              |
| 2:C:764:GLU:HB3   | 2:C:766:GLU:OE2  | 2.04                     | 0.58              |
| 2:C:988:VAL:N     | 3:D:948:THR:HG21 | 2.18                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1147:ARG:O    | 3:D:1166:LEU:HG   | 2.04                     | 0.58              |
| 3:D:1256:LEU:HB3  | 3:D:1257:PRO:HD3  | 1.86                     | 0.58              |
| 3:D:142:LEU:HD23  | 3:D:146:PRO:HA    | 1.85                     | 0.58              |
| 3:D:1463:LYS:O    | 3:D:1467:ILE:HG22 | 2.04                     | 0.58              |
| 3:D:1478:SER:C    | 3:D:1482:ARG:HG3  | 2.24                     | 0.58              |
| 3:D:528:VAL:HG12  | 3:D:529:GLN:O     | 2.04                     | 0.58              |
| 3:D:653:PHE:CD1   | 3:D:653:PHE:N     | 2.71                     | 0.58              |
| 2:C:676:ILE:CD1   | 3:D:949:ILE:HB    | 2.34                     | 0.58              |
| 1:L:33:GLY:O      | 1:L:195:LEU:HD22  | 2.03                     | 0.58              |
| 2:M:884:GLN:O     | 2:M:887:GLU:HB3   | 2.04                     | 0.58              |
| 3:N:1159:ARG:O    | 3:N:1160:LEU:HD23 | 2.04                     | 0.58              |
| 3:N:1182:GLU:HG2  | 3:N:1182:GLU:O    | 2.02                     | 0.58              |
| 3:N:167:GLU:C     | 3:N:394:LEU:HD12  | 2.24                     | 0.58              |
| 3:N:230:TRP:HE1   | 3:N:233:LYS:CG    | 2.16                     | 0.58              |
| 3:N:245:LEU:CA    | 3:N:309:GLY:H     | 2.07                     | 0.58              |
| 3:N:131:LYS:HB2   | 3:N:456:MET:HE2   | 1.85                     | 0.58              |
| 3:N:653:PHE:CD1   | 3:N:653:PHE:N     | 2.70                     | 0.58              |
| 1:A:109:VAL:HG12  | 1:A:129:ILE:HB    | 1.86                     | 0.58              |
| 2:C:73:LEU:HB3    | 2:C:94:LEU:HA     | 1.85                     | 0.58              |
| 3:D:1153:VAL:HG12 | 3:D:1155:VAL:HG23 | 1.86                     | 0.58              |
| 3:D:153:LEU:HG    | 3:D:154:THR:N     | 2.19                     | 0.58              |
| 3:D:325:GLU:CG    | 3:D:332:TYR:HB3   | 2.34                     | 0.58              |
| 3:D:465:LEU:HD22  | 3:D:509:PRO:HB2   | 1.84                     | 0.58              |
| 3:D:563:PRO:O     | 3:D:565:ILE:N     | 2.36                     | 0.58              |
| 4:E:39:VAL:CG1    | 4:E:72:ARG:HB3    | 2.33                     | 0.58              |
| 5:F:94:LEU:HD11   | 5:F:190:ALA:HB3   | 1.86                     | 0.58              |
| 2:M:939:ARG:HD2   | 2:M:982:PRO:CD    | 2.33                     | 0.58              |
| 3:N:1067:VAL:HG13 | 3:N:1068:LEU:H    | 1.68                     | 0.58              |
| 3:N:1446:VAL:O    | 3:N:1449:GLU:HG2  | 2.03                     | 0.58              |
| 3:N:172:PRO:HB2   | 3:N:175:VAL:HG21  | 1.86                     | 0.58              |
| 3:N:456:MET:N     | 3:N:456:MET:SD    | 2.77                     | 0.58              |
| 2:M:1031:ARG:HB2  | 3:N:622:ARG:NH1   | 2.18                     | 0.58              |
| 3:N:858:VAL:CG1   | 3:N:859:ASP:N     | 2.67                     | 0.58              |
| 5:P:355:GLU:OE1   | 5:P:356:LYS:N     | 2.36                     | 0.58              |
| 1:A:80:LEU:O      | 1:A:83:LYS:HB2    | 2.04                     | 0.58              |
| 2:C:639:GLN:HA    | 2:C:657:ASP:O     | 2.03                     | 0.58              |
| 2:C:949:LYS:HZ3   | 3:D:796:ARG:NH1   | 2.02                     | 0.58              |
| 2:C:994:ILE:HG22  | 2:C:995:MET:N     | 2.18                     | 0.58              |
| 3:D:1104:GLU:O    | 3:D:1108:ARG:NH2  | 2.37                     | 0.58              |
| 3:D:288:MET:SD    | 3:D:305:ALA:HB1   | 2.43                     | 0.58              |
| 3:D:165:LYS:O     | 3:D:396:VAL:HG23  | 2.02                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:801:GLY:CA    | 3:D:830:ALA:HB3   | 2.34                     | 0.58              |
| 3:D:953:ASP:O     | 3:D:955:VAL:HG23  | 2.04                     | 0.58              |
| 2:M:1037:VAL:HG13 | 2:M:1049:LEU:HD21 | 1.86                     | 0.58              |
| 2:M:432:ARG:HG3   | 2:M:433:THR:N     | 2.19                     | 0.58              |
| 2:M:596:TYR:HA    | 2:M:653:ASP:O     | 2.04                     | 0.58              |
| 2:M:807:ARG:C     | 2:M:809:GLY:N     | 2.51                     | 0.58              |
| 3:N:1066:THR:O    | 3:N:1067:VAL:C    | 2.42                     | 0.58              |
| 3:N:135:LEU:CD1   | 3:N:148:GLU:HB2   | 2.32                     | 0.58              |
| 3:N:153:LEU:HD21  | 3:N:158:TYR:CA    | 2.34                     | 0.58              |
| 3:N:266:GLU:HB3   | 3:N:286:VAL:HG22  | 1.84                     | 0.58              |
| 3:N:587:ARG:NH1   | 3:N:587:ARG:HB3   | 2.19                     | 0.58              |
| 3:N:656:PHE:CZ    | 3:N:751:LEU:HD23  | 2.39                     | 0.58              |
| 5:P:95:THR:O      | 5:P:98:GLU:N      | 2.37                     | 0.58              |
| 2:C:523:ILE:O     | 2:C:524:VAL:HG13  | 2.03                     | 0.57              |
| 3:D:222:GLY:HA2   | 3:D:333:LEU:O     | 2.03                     | 0.57              |
| 3:D:406:ASP:HB2   | 3:D:423:ASP:C     | 2.24                     | 0.57              |
| 3:D:418:GLY:O     | 3:D:428:LYS:HE2   | 2.04                     | 0.57              |
| 1:K:143:ARG:HH11  | 1:K:158:ILE:HG23  | 1.68                     | 0.57              |
| 1:K:45:LEU:HB2    | 2:M:856:GLU:HG3   | 1.86                     | 0.57              |
| 1:K:76:VAL:HA     | 1:K:79:ILE:CD1    | 2.30                     | 0.57              |
| 1:L:28:LEU:HD22   | 1:L:32:PHE:HB2    | 1.86                     | 0.57              |
| 2:M:23:VAL:HG12   | 2:M:121:MET:HE1   | 1.85                     | 0.57              |
| 2:M:23:VAL:HG23   | 2:M:24:GLU:N      | 2.19                     | 0.57              |
| 2:M:261:ILE:CG2   | 2:M:262:ALA:H     | 2.17                     | 0.57              |
| 2:M:327:HIS:CE1   | 2:M:488:ALA:HB1   | 2.39                     | 0.57              |
| 2:M:833:LEU:HD11  | 2:M:837:ASP:HB2   | 1.86                     | 0.57              |
| 3:N:1489:GLN:NE2  | 4:O:73:LEU:N      | 2.52                     | 0.57              |
| 3:N:266:GLU:HB3   | 3:N:286:VAL:HG21  | 1.83                     | 0.57              |
| 3:N:502:PHE:CE2   | 3:N:1452:ILE:HG23 | 2.39                     | 0.57              |
| 3:N:930:LEU:HG    | 3:N:934:LEU:HD11  | 1.86                     | 0.57              |
| 5:P:171:LYS:O     | 5:P:174:LEU:HB3   | 2.03                     | 0.57              |
| 5:P:262:VAL:C     | 5:P:264:MET:N     | 2.54                     | 0.57              |
| 5:P:379:ARG:HB2   | 5:P:379:ARG:HH11  | 1.68                     | 0.57              |
| 5:P:382:THR:HG22  | 5:P:394:ARG:HA    | 1.85                     | 0.57              |
| 2:C:987:ILE:CA    | 3:D:948:THR:HG21  | 2.34                     | 0.57              |
| 3:D:284:LEU:HD12  | 3:D:290:PRO:CB    | 2.28                     | 0.57              |
| 3:D:474:GLU:OE2   | 3:D:475:LYS:HG3   | 2.04                     | 0.57              |
| 3:D:499:VAL:HG12  | 3:D:503:LEU:HD12  | 1.84                     | 0.57              |
| 3:D:875:THR:CG2   | 3:D:879:ARG:HG3   | 2.34                     | 0.57              |
| 4:E:25:LYS:HA     | 4:E:28:GLN:CD     | 2.23                     | 0.57              |
| 4:E:37:ASN:HA     | 4:E:93:TYR:CE2    | 2.38                     | 0.57              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:413:SER:HA   | 5:F:416:ARG:NH2   | 2.19                     | 0.57              |
| 1:L:36:LEU:O     | 1:L:40:LEU:HD12   | 2.04                     | 0.57              |
| 3:N:1028:ALA:O   | 3:N:1029:ARG:HB2  | 2.03                     | 0.57              |
| 3:N:1445:HIS:O   | 3:N:1449:GLU:HG2  | 2.04                     | 0.57              |
| 3:N:269:PHE:HE2  | 3:N:271:VAL:HG22  | 1.68                     | 0.57              |
| 3:N:661:MET:SD   | 3:N:673:ALA:HB1   | 2.44                     | 0.57              |
| 3:N:788:GLY:HA3  | 3:N:938:GLY:O     | 2.04                     | 0.57              |
| 2:C:182:VAL:HG22 | 2:C:221:LEU:HA    | 1.86                     | 0.57              |
| 2:C:39:ARG:O     | 2:C:40:GLU:HB2    | 2.04                     | 0.57              |
| 2:C:517:ARG:H    | 2:C:520:GLU:HB2   | 1.68                     | 0.57              |
| 3:D:1085:ALA:HA  | 3:D:1088:THR:HG22 | 1.85                     | 0.57              |
| 3:D:1445:HIS:O   | 3:D:1449:GLU:HG2  | 2.04                     | 0.57              |
| 3:D:433:GLY:O    | 3:D:434:ARG:HD2   | 2.04                     | 0.57              |
| 3:D:450:TYR:CE2  | 3:D:452:ILE:HG22  | 2.39                     | 0.57              |
| 3:D:608:SER:HB2  | 3:D:614:PHE:CD1   | 2.39                     | 0.57              |
| 3:D:800:LYS:NZ   | 3:D:826:PRO:HD3   | 2.19                     | 0.57              |
| 4:E:40:LEU:HD21  | 4:E:44:GLU:CB     | 2.34                     | 0.57              |
| 4:E:57:ASP:O     | 4:E:63:TRP:NE1    | 2.37                     | 0.57              |
| 5:F:393:THR:HG22 | 5:F:394:ARG:N     | 2.19                     | 0.57              |
| 1:L:144:VAL:HG12 | 1:L:145:ASP:N     | 2.19                     | 0.57              |
| 1:L:90:LEU:HG    | 1:L:119:ASP:O     | 2.05                     | 0.57              |
| 2:M:1069:ALA:HB1 | 2:M:1075:ASP:O    | 2.04                     | 0.57              |
| 2:M:289:THR:O    | 2:M:290:LEU:HD23  | 2.03                     | 0.57              |
| 2:M:31:GLN:HA    | 2:M:35:PRO:HG2    | 1.87                     | 0.57              |
| 2:M:38:LYS:HG3   | 2:M:39:ARG:N      | 2.16                     | 0.57              |
| 3:N:106:LYS:HB3  | 3:N:586:ARG:NH1   | 2.18                     | 0.57              |
| 3:N:1149:LEU:HG  | 3:N:1162:GLU:HA   | 1.86                     | 0.57              |
| 3:N:1333:HIS:HA  | 3:N:1421:LEU:HD23 | 1.84                     | 0.57              |
| 3:N:1382:THR:O   | 3:N:1389:LEU:HD21 | 2.05                     | 0.57              |
| 3:N:399:ARG:HB3  | 3:N:401:TYR:CE1   | 2.36                     | 0.57              |
| 5:P:412:GLU:HA   | 5:P:412:GLU:OE2   | 2.03                     | 0.57              |
| 5:P:356:LYS:HD3  | 5:P:417:LYS:NZ    | 2.19                     | 0.57              |
| 1:A:10:VAL:HG12  | 1:A:12:THR:HG23   | 1.87                     | 0.57              |
| 1:B:41:ARG:O     | 1:B:44:LEU:HB2    | 2.05                     | 0.57              |
| 2:C:203:ASP:OD1  | 2:C:205:GLU:HB3   | 2.03                     | 0.57              |
| 2:C:375:SER:C    | 2:C:377:PRO:HD2   | 2.25                     | 0.57              |
| 2:C:773:LEU:O    | 2:C:777:ILE:HG13  | 2.04                     | 0.57              |
| 2:C:914:ILE:HD12 | 2:C:914:ILE:H     | 1.68                     | 0.57              |
| 3:D:1344:VAL:O   | 3:D:1347:TYR:HB3  | 2.04                     | 0.57              |
| 3:D:458:ALA:O    | 3:D:459:GLU:C     | 2.41                     | 0.57              |
| 3:D:86:ARG:O     | 3:D:522:PRO:HD2   | 2.04                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:811:GLU:O     | 3:D:815:ALA:CB    | 2.50                     | 0.57              |
| 2:C:1083:GLU:CD   | 3:D:88:TYR:HH     | 2.07                     | 0.57              |
| 3:D:903:ASP:O     | 3:D:904:VAL:HG13  | 2.03                     | 0.57              |
| 1:L:137:ARG:HG2   | 1:L:137:ARG:NH1   | 2.17                     | 0.57              |
| 1:L:85:LEU:HD12   | 1:L:86:VAL:N      | 2.19                     | 0.57              |
| 2:M:128:ILE:HA    | 2:M:132:ALA:O     | 2.04                     | 0.57              |
| 2:M:198:ARG:HH11  | 2:M:203:ASP:N     | 2.02                     | 0.57              |
| 2:M:203:ASP:CB    | 2:M:228:ALA:O     | 2.51                     | 0.57              |
| 2:M:41:ASN:HA     | 2:M:45:GLN:CB     | 2.32                     | 0.57              |
| 2:M:601:GLY:O     | 2:M:648:ARG:HA    | 2.04                     | 0.57              |
| 2:M:708:TYR:O     | 2:M:824:ARG:HA    | 2.05                     | 0.57              |
| 3:N:1120:VAL:CB   | 3:N:1144:LEU:HD21 | 2.34                     | 0.57              |
| 3:N:1167:SER:O    | 3:N:1170:ASP:HB2  | 2.03                     | 0.57              |
| 3:N:793:THR:HG21  | 3:N:906:GLN:CG    | 2.34                     | 0.57              |
| 3:N:854:ALA:C     | 3:N:856:GLY:H     | 2.08                     | 0.57              |
| 3:N:986:ARG:O     | 3:N:987:GLU:C     | 2.42                     | 0.57              |
| 5:P:278:LEU:O     | 5:P:279:GLN:C     | 2.43                     | 0.57              |
| 3:N:537:THR:HA    | 5:P:317:LEU:HD11  | 1.87                     | 0.57              |
| 2:C:479:VAL:HG23  | 2:C:506:ASN:O     | 2.04                     | 0.57              |
| 2:C:630:ARG:HG3   | 2:C:634:GLY:HA2   | 1.85                     | 0.57              |
| 2:C:713:ARG:HA    | 2:C:818:GLY:O     | 2.04                     | 0.57              |
| 2:C:878:SER:C     | 2:C:879:ARG:HD2   | 2.25                     | 0.57              |
| 2:C:910:LYS:HE3   | 2:C:912:PRO:HB2   | 1.86                     | 0.57              |
| 3:D:1278:ASP:HA   | 3:D:1319:VAL:O    | 2.05                     | 0.57              |
| 3:D:1468:LEU:HD23 | 3:D:1470:ARG:HB2  | 1.85                     | 0.57              |
| 3:D:247:GLU:HA    | 3:D:308:LYS:HZ3   | 1.68                     | 0.57              |
| 3:D:227:LEU:HD11  | 3:D:327:GLU:N     | 2.19                     | 0.57              |
| 3:D:540:LEU:O     | 3:D:541:ASN:C     | 2.43                     | 0.57              |
| 3:D:800:LYS:CE    | 3:D:800:LYS:H     | 2.16                     | 0.57              |
| 3:D:966:GLU:HA    | 3:D:969:ARG:NE    | 2.20                     | 0.57              |
| 4:E:26:ARG:HH21   | 4:E:38:THR:HA     | 1.70                     | 0.57              |
| 3:D:674:ARG:NH2   | 5:F:342:VAL:HG13  | 2.19                     | 0.57              |
| 1:K:184:THR:O     | 1:K:192:LEU:HB2   | 2.05                     | 0.57              |
| 2:M:173:ASP:O     | 2:M:174:LEU:HD23  | 2.03                     | 0.57              |
| 2:M:205:GLU:HA    | 2:M:209:ARG:HH11  | 1.70                     | 0.57              |
| 2:M:576:ALA:O     | 2:M:900:ARG:NH1   | 2.37                     | 0.57              |
| 2:M:971:LYS:HA    | 2:M:988:VAL:HA    | 1.86                     | 0.57              |
| 3:N:126:VAL:O     | 3:N:132:TYR:HD1   | 1.88                     | 0.57              |
| 3:N:339:TRP:CH2   | 3:N:341:GLU:HG3   | 2.40                     | 0.57              |
| 3:N:704:ARG:HB2   | 3:N:745:MET:SD    | 2.44                     | 0.57              |
| 3:N:881:LEU:HD21  | 3:N:941:PHE:HZ    | 1.69                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:180:GLY:O     | 5:P:183:ALA:HB3   | 2.05                     | 0.57              |
| 1:A:111:ALA:O     | 1:A:113:ASP:N     | 2.38                     | 0.57              |
| 2:C:198:ARG:NE    | 2:C:231:PRO:HG3   | 2.19                     | 0.57              |
| 2:C:444:PRO:HG3   | 2:C:452:ILE:HB    | 1.85                     | 0.57              |
| 2:C:706:GLU:HG3   | 2:C:708:TYR:CE1   | 2.39                     | 0.57              |
| 2:C:715:THR:HG22  | 2:C:717:LEU:H     | 1.68                     | 0.57              |
| 2:C:799:ILE:O     | 2:C:799:ILE:HG13  | 2.04                     | 0.57              |
| 2:C:882:LEU:O     | 2:C:885:ILE:N     | 2.38                     | 0.57              |
| 3:D:1104:GLU:N    | 3:D:1104:GLU:OE1  | 2.37                     | 0.57              |
| 3:D:1311:LEU:HG   | 3:D:1312:LEU:N    | 2.20                     | 0.57              |
| 3:D:1434:TRP:CE3  | 3:D:1457:ASP:HB2  | 2.40                     | 0.57              |
| 2:C:1046:ALA:HA   | 3:D:1472:ILE:HB   | 1.85                     | 0.57              |
| 3:D:160:GLU:CD    | 3:D:165:LYS:HE2   | 2.25                     | 0.57              |
| 3:D:546:ARG:O     | 3:D:549:ASN:HB2   | 2.05                     | 0.57              |
| 3:D:80:VAL:O      | 3:D:81:THR:HG23   | 2.05                     | 0.57              |
| 3:D:965:GLU:O     | 3:D:967:ALA:N     | 2.37                     | 0.57              |
| 4:E:19:LEU:O      | 4:E:22:VAL:HB     | 2.04                     | 0.57              |
| 4:E:86:GLN:O      | 4:E:90:GLU:N      | 2.37                     | 0.57              |
| 5:F:192:LEU:HB3   | 11:F:424:HOH:O    | 2.05                     | 0.57              |
| 3:N:1046:GLN:CB   | 3:N:1052:THR:HA   | 2.34                     | 0.57              |
| 3:N:1383:ASP:HB3  | 3:N:1416:ALA:H    | 1.69                     | 0.57              |
| 3:N:217:LYS:HB2   | 3:N:339:TRP:CD1   | 2.39                     | 0.57              |
| 3:N:133:ILE:HG23  | 3:N:456:MET:SD    | 2.45                     | 0.57              |
| 3:N:522:PRO:CA    | 3:N:525:ARG:NH1   | 2.68                     | 0.57              |
| 3:N:654:LYS:HB3   | 3:N:655:PRO:CD    | 2.28                     | 0.57              |
| 5:P:295:MET:HG3   | 5:P:299:TRP:CD2   | 2.39                     | 0.57              |
| 5:P:401:GLU:O     | 5:P:405:LEU:HG    | 2.05                     | 0.57              |
| 1:A:57:TYR:O      | 1:A:140:MET:HB2   | 2.05                     | 0.57              |
| 1:B:61:VAL:HG22   | 1:B:62:LEU:N      | 2.20                     | 0.57              |
| 2:C:101:ILE:HD13  | 2:C:107:LEU:HD22  | 1.86                     | 0.57              |
| 2:C:603:VAL:HG21  | 2:C:647:GLN:HB3   | 1.85                     | 0.57              |
| 2:C:805:ARG:NE    | 2:C:807:ARG:HH21  | 2.02                     | 0.57              |
| 3:D:1048:PRO:HG3  | 3:D:1075:HIS:CD2  | 2.34                     | 0.57              |
| 3:D:1107:VAL:HB   | 3:D:1219:GLU:H    | 1.69                     | 0.57              |
| 3:D:1156:LEU:HD12 | 3:D:1173:LEU:HD11 | 1.87                     | 0.57              |
| 3:D:119:SER:N     | 3:D:123:LEU:HB2   | 2.20                     | 0.57              |
| 3:D:223:LEU:HG    | 3:D:224:ARG:N     | 2.14                     | 0.57              |
| 3:D:671:LYS:HE2   | 3:D:675:ARG:HD3   | 1.87                     | 0.57              |
| 3:D:844:ALA:O     | 3:D:867:ARG:HD2   | 2.04                     | 0.57              |
| 5:F:163:LEU:HA    | 5:F:166:LEU:CD1   | 2.35                     | 0.57              |
| 1:K:124:ASN:HB3   | 1:K:127:LEU:HB2   | 1.87                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:25:LEU:HD21  | 1:L:224:TYR:HB2  | 1.86                     | 0.57              |
| 2:M:604:ALA:HB3  | 2:M:612:VAL:O    | 2.05                     | 0.57              |
| 3:N:125:GLN:HG3  | 3:N:126:VAL:N    | 2.19                     | 0.57              |
| 3:N:219:GLU:HG2  | 3:N:220:ARG:N    | 2.15                     | 0.57              |
| 3:N:241:ILE:HG12 | 3:N:312:ARG:CG   | 2.32                     | 0.57              |
| 3:N:257:GLY:HA2  | 3:N:274:ARG:CA   | 2.32                     | 0.57              |
| 3:N:252:ARG:NE   | 3:N:300:LYS:HA   | 2.16                     | 0.57              |
| 5:P:213:ILE:HG22 | 5:P:217:ASN:ND2  | 2.19                     | 0.57              |
| 5:P:352:GLU:O    | 5:P:354:LEU:N    | 2.37                     | 0.57              |
| 2:C:194:VAL:CA   | 2:C:197:LEU:HG   | 2.35                     | 0.57              |
| 2:C:148:PHE:N    | 2:C:323:ASP:OD2  | 2.31                     | 0.57              |
| 2:C:415:PRO:CB   | 2:C:418:LEU:HB2  | 2.29                     | 0.57              |
| 2:C:488:ALA:O    | 2:C:491:GLU:HB3  | 2.05                     | 0.57              |
| 2:C:596:TYR:HA   | 2:C:653:ASP:O    | 2.05                     | 0.57              |
| 2:C:597:ALA:N    | 2:C:653:ASP:O    | 2.38                     | 0.57              |
| 2:C:841:ASN:HD21 | 2:C:845:ASN:CB   | 2.18                     | 0.57              |
| 3:D:108:VAL:CG1  | 3:D:109:PRO:HA   | 2.34                     | 0.57              |
| 3:D:1293:PHE:CZ  | 3:D:1300:SER:HB3 | 2.40                     | 0.57              |
| 3:D:537:THR:C    | 5:F:317:LEU:HG   | 2.24                     | 0.57              |
| 3:D:591:VAL:HB   | 3:D:598:ARG:O    | 2.05                     | 0.57              |
| 3:D:5:VAL:HG22   | 3:D:6:ARG:N      | 2.19                     | 0.57              |
| 3:D:800:LYS:HD2  | 3:D:800:LYS:H    | 1.69                     | 0.57              |
| 3:D:924:MET:HG2  | 4:E:7:ASP:OD2    | 2.05                     | 0.57              |
| 3:D:924:MET:O    | 3:D:927:THR:HB   | 2.05                     | 0.57              |
| 5:F:277:GLN:HA   | 5:F:280:GLN:CD   | 2.25                     | 0.57              |
| 5:F:386:VAL:CG2  | 5:F:387:GLY:H    | 2.16                     | 0.57              |
| 1:K:100:LEU:HD22 | 1:K:102:LYS:HE3  | 1.87                     | 0.57              |
| 2:M:369:PRO:HD2  | 2:M:371:LYS:HD2  | 1.87                     | 0.57              |
| 2:M:53:PRO:HB3   | 2:M:67:ASP:CG    | 2.25                     | 0.57              |
| 3:N:284:LEU:HD12 | 3:N:290:PRO:HB3  | 1.85                     | 0.57              |
| 3:N:584:ASN:ND2  | 3:N:590:PRO:HG2  | 2.18                     | 0.57              |
| 3:N:771:SER:CB   | 3:N:778:LEU:HD22 | 2.34                     | 0.57              |
| 3:N:858:VAL:CG1  | 3:N:859:ASP:H    | 2.17                     | 0.57              |
| 4:O:25:LYS:HA    | 4:O:28:GLN:NE2   | 2.20                     | 0.57              |
| 4:O:82:GLU:O     | 4:O:85:LEU:HG    | 2.04                     | 0.57              |
| 1:A:107:LYS:NZ   | 1:A:108:GLU:O    | 2.37                     | 0.57              |
| 1:A:39:PRO:HG3   | 1:B:39:PRO:CG    | 2.30                     | 0.57              |
| 1:B:84:GLU:HB2   | 1:B:127:LEU:HD21 | 1.87                     | 0.57              |
| 2:C:1052:MET:O   | 2:C:1056:LYS:HB2 | 2.05                     | 0.57              |
| 2:C:122:THR:HB   | 2:C:124:ASP:OD1  | 2.05                     | 0.57              |
| 2:C:224:GLU:HB3  | 2:C:227:PHE:CD1  | 2.40                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:343:GLN:HG2  | 2:C:385:PHE:HB2   | 1.87                     | 0.57              |
| 2:C:345:ARG:O    | 2:C:348:LEU:HB3   | 2.05                     | 0.57              |
| 2:C:41:ASN:O     | 2:C:43:GLY:N      | 2.38                     | 0.57              |
| 2:C:882:LEU:O    | 2:C:883:GLY:C     | 2.43                     | 0.57              |
| 3:D:1464:GLU:O   | 3:D:1467:ILE:HG22 | 2.04                     | 0.57              |
| 5:F:189:GLU:HA   | 5:F:192:LEU:CD1   | 2.33                     | 0.57              |
| 1:K:1:MET:O      | 1:K:1:MET:SD      | 2.62                     | 0.57              |
| 1:K:98:THR:CG2   | 1:K:141:GLU:HB3   | 2.35                     | 0.57              |
| 1:L:206:THR:HG22 | 1:L:208:LEU:H     | 1.70                     | 0.57              |
| 1:K:9:PRO:HD2    | 1:L:224:TYR:CE1   | 2.40                     | 0.57              |
| 1:L:5:LYS:C      | 1:L:7:LYS:H       | 2.07                     | 0.57              |
| 2:M:380:ALA:O    | 2:M:381:ALA:C     | 2.43                     | 0.57              |
| 2:M:430:VAL:HG13 | 2:M:430:VAL:O     | 2.04                     | 0.57              |
| 2:M:488:ALA:O    | 2:M:491:GLU:HB3   | 2.05                     | 0.57              |
| 2:M:50:GLU:C     | 2:M:52:PHE:N      | 2.58                     | 0.57              |
| 2:M:605:LYS:CB   | 2:M:610:ARG:HH21  | 2.16                     | 0.57              |
| 2:M:69:LEU:HD23  | 2:M:70:GLU:HG3    | 1.87                     | 0.57              |
| 3:N:1042:ARG:HG2 | 3:N:1042:ARG:HH11 | 1.69                     | 0.57              |
| 3:N:457:GLY:O    | 3:N:461:ILE:HG12  | 2.05                     | 0.57              |
| 3:N:45:PHE:O     | 3:N:47:GLU:N      | 2.37                     | 0.57              |
| 3:N:653:PHE:O    | 3:N:654:LYS:C     | 2.42                     | 0.57              |
| 3:N:732:VAL:C    | 3:N:734:GLU:N     | 2.57                     | 0.57              |
| 3:N:788:GLY:H    | 3:N:942:SER:HB3   | 1.68                     | 0.57              |
| 1:A:209:GLU:HA   | 1:A:212:ASN:ND2   | 2.20                     | 0.57              |
| 2:C:513:VAL:O    | 2:C:523:ILE:HA    | 2.05                     | 0.57              |
| 2:C:69:LEU:CD2   | 2:C:70:GLU:HG3    | 2.34                     | 0.57              |
| 2:C:726:ILE:C    | 2:C:728:HIS:H     | 2.08                     | 0.57              |
| 3:D:156:GLU:OE2  | 3:D:156:GLU:N     | 2.38                     | 0.57              |
| 3:D:223:LEU:CG   | 3:D:224:ARG:H     | 2.13                     | 0.57              |
| 3:D:99:ALA:O     | 3:D:514:LEU:N     | 2.38                     | 0.57              |
| 3:D:530:VAL:HG22 | 3:D:534:ARG:O     | 2.04                     | 0.57              |
| 3:D:821:VAL:C    | 3:D:823:LEU:H     | 2.07                     | 0.57              |
| 5:F:245:GLN:CA   | 5:F:245:GLN:HE21  | 2.13                     | 0.57              |
| 5:F:383:LEU:CD2  | 5:F:394:ARG:HD3   | 2.34                     | 0.57              |
| 1:K:86:VAL:HG21  | 1:K:202:ASP:HB2   | 1.86                     | 0.57              |
| 1:K:41:ARG:HA    | 1:K:44:LEU:HD12   | 1.87                     | 0.57              |
| 1:L:163:ASN:O    | 1:L:165:ILE:HG13  | 2.05                     | 0.57              |
| 1:L:38:ASN:O     | 1:L:41:ARG:HB3    | 2.04                     | 0.57              |
| 2:M:193:LEU:CD2  | 2:M:307:LEU:HD22  | 2.34                     | 0.57              |
| 2:M:352:ALA:HA   | 2:M:355:VAL:CG1   | 2.33                     | 0.57              |
| 3:N:1402:ALA:HA  | 3:N:1415:VAL:HG21 | 1.86                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:673:ALA:CA    | 3:N:676:MET:HB3   | 2.34                     | 0.57              |
| 3:N:984:THR:HG22  | 3:N:987:GLU:HB2   | 1.87                     | 0.57              |
| 1:A:124:ASN:HB2   | 1:A:127:LEU:HB2   | 1.87                     | 0.56              |
| 1:A:49:PRO:CA     | 1:A:148:VAL:HG12  | 2.35                     | 0.56              |
| 1:A:14:ARG:HG3    | 1:A:14:ARG:O      | 2.05                     | 0.56              |
| 2:C:504:GLU:O     | 2:C:506:ASN:N     | 2.38                     | 0.56              |
| 2:C:654:LEU:CD1   | 2:C:655:LEU:H     | 2.12                     | 0.56              |
| 2:C:914:ILE:HD12  | 2:C:914:ILE:N     | 2.20                     | 0.56              |
| 2:C:1039:ALA:HA   | 3:D:1227:GLN:HE22 | 1.70                     | 0.56              |
| 3:D:224:ARG:NH1   | 3:D:332:TYR:CD1   | 2.73                     | 0.56              |
| 3:D:50:PHE:CD2    | 3:D:522:PRO:HD3   | 2.40                     | 0.56              |
| 3:D:827:ILE:HG23  | 3:D:837:GLY:CA    | 2.34                     | 0.56              |
| 5:F:261:PRO:HB2   | 5:F:264:MET:HG2   | 1.87                     | 0.56              |
| 1:K:110:LYS:HB2   | 1:K:112:ARG:CG    | 2.28                     | 0.56              |
| 1:K:39:PRO:O      | 1:K:42:ARG:HB2    | 2.05                     | 0.56              |
| 2:M:122:THR:HG22  | 2:M:123:GLU:N     | 2.19                     | 0.56              |
| 2:M:128:ILE:C     | 2:M:129:ILE:HD13  | 2.25                     | 0.56              |
| 2:M:926:PHE:O     | 2:M:929:ARG:N     | 2.31                     | 0.56              |
| 3:N:119:SER:N     | 3:N:123:LEU:HB2   | 2.20                     | 0.56              |
| 3:N:1292:VAL:HG12 | 3:N:1293:PHE:N    | 2.19                     | 0.56              |
| 3:N:1479:ASP:HA   | 3:N:1483:PHE:HE1  | 1.70                     | 0.56              |
| 3:N:250:LEU:HD13  | 3:N:306:GLU:HG2   | 1.86                     | 0.56              |
| 3:N:662:GLU:HA    | 3:N:667:ALA:O     | 2.03                     | 0.56              |
| 5:P:245:GLN:NE2   | 5:P:245:GLN:CA    | 2.68                     | 0.56              |
| 5:P:253:ASP:HA    | 5:P:259:ARG:HH12  | 1.69                     | 0.56              |
| 3:N:30:GLU:HG3    | 5:P:259:ARG:HB2   | 1.86                     | 0.56              |
| 2:C:293:PHE:HD1   | 2:C:294:GLU:HG3   | 1.68                     | 0.56              |
| 2:C:577:PRO:HG3   | 2:C:993:PHE:CG    | 2.40                     | 0.56              |
| 3:D:1445:HIS:O    | 3:D:1446:VAL:C    | 2.44                     | 0.56              |
| 3:D:186:VAL:HG12  | 3:D:187:LYS:H     | 1.68                     | 0.56              |
| 3:D:225:LEU:HD22  | 3:D:243:ALA:HB2   | 1.87                     | 0.56              |
| 3:D:257:GLY:N     | 3:D:272:LEU:HD22  | 2.20                     | 0.56              |
| 3:D:970:LYS:HA    | 3:D:973:GLN:NE2   | 2.20                     | 0.56              |
| 4:E:50:THR:O      | 4:E:55:PHE:CE1    | 2.58                     | 0.56              |
| 5:F:381:HIS:H     | 5:F:385:GLU:CD    | 2.09                     | 0.56              |
| 1:K:64:GLU:HG3    | 1:K:64:GLU:O      | 2.04                     | 0.56              |
| 2:M:91:GLN:HB2    | 2:M:118:ILE:C     | 2.26                     | 0.56              |
| 2:M:265:ARG:HD2   | 2:M:268:ASP:HA    | 1.85                     | 0.56              |
| 2:M:582:GLY:N     | 2:M:584:GLU:OE2   | 2.29                     | 0.56              |
| 3:N:1093:TYR:O    | 3:N:1097:LYS:HG2  | 2.04                     | 0.56              |
| 3:N:188:GLY:H     | 3:N:198:ARG:CA    | 2.17                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:22:SER:C     | 3:N:24:GLY:H      | 2.08                     | 0.56              |
| 3:N:685:ASP:O    | 3:N:687:VAL:N     | 2.37                     | 0.56              |
| 5:P:308:LEU:H    | 5:P:308:LEU:HD23  | 1.69                     | 0.56              |
| 1:B:13:VAL:CG2   | 1:B:14:ARG:N      | 2.67                     | 0.56              |
| 1:B:95:GLN:HE22  | 1:B:146:ARG:NH1   | 2.02                     | 0.56              |
| 2:C:285:LEU:HD12 | 2:C:289:THR:O     | 2.04                     | 0.56              |
| 2:C:54:ILE:HD12  | 2:C:352:ALA:HB1   | 1.87                     | 0.56              |
| 2:C:55:GLU:CD    | 2:C:57:GLU:HB3    | 2.26                     | 0.56              |
| 3:D:1038:LEU:O   | 3:D:1060:SER:HB2  | 2.05                     | 0.56              |
| 3:D:1412:LYS:O   | 3:D:1414:PRO:HD3  | 2.05                     | 0.56              |
| 3:D:428:LYS:HG2  | 3:D:429:SER:H     | 1.69                     | 0.56              |
| 3:D:556:LYS:O    | 3:D:560:GLN:N     | 2.38                     | 0.56              |
| 3:D:800:LYS:HE3  | 3:D:826:PRO:HD3   | 1.86                     | 0.56              |
| 5:F:132:ARG:HB3  | 5:F:136:LEU:HD11  | 1.87                     | 0.56              |
| 5:F:210:LEU:HA   | 5:F:213:ILE:CD1   | 2.16                     | 0.56              |
| 1:K:176:ARG:NE   | 2:M:865:THR:HG22  | 2.20                     | 0.56              |
| 2:M:101:ILE:HG23 | 2:M:107:LEU:HD23  | 1.88                     | 0.56              |
| 2:M:508:ILE:HG22 | 2:M:509:ALA:N     | 2.20                     | 0.56              |
| 2:M:641:PRO:O    | 2:M:642:ARG:HD3   | 2.06                     | 0.56              |
| 2:M:745:ILE:HG22 | 2:M:746:GLY:N     | 2.20                     | 0.56              |
| 2:M:772:ARG:NH2  | 5:P:379:ARG:HG3   | 2.20                     | 0.56              |
| 2:M:853:LEU:HB2  | 2:M:858:MET:CE    | 2.35                     | 0.56              |
| 3:N:1094:LEU:HG  | 3:N:1095:THR:N    | 2.19                     | 0.56              |
| 3:N:1401:GLU:H   | 3:N:1401:GLU:CD   | 2.09                     | 0.56              |
| 3:N:657:LEU:HG   | 3:N:661:MET:CE    | 2.34                     | 0.56              |
| 3:N:939:PHE:O    | 3:N:941:PHE:N     | 2.38                     | 0.56              |
| 3:N:95:LEU:HB3   | 3:N:97:THR:O      | 2.04                     | 0.56              |
| 3:N:350:HIS:ND1  | 5:P:232:ARG:NH2   | 2.52                     | 0.56              |
| 1:A:206:THR:HG23 | 1:A:207:PRO:HD2   | 1.86                     | 0.56              |
| 1:A:9:PRO:HB2    | 1:A:25:LEU:HD11   | 1.87                     | 0.56              |
| 2:C:1014:SER:CA  | 2:C:1021:LEU:HD22 | 2.35                     | 0.56              |
| 2:C:352:ALA:HA   | 2:C:355:VAL:CG1   | 2.33                     | 0.56              |
| 2:C:413:LEU:CA   | 2:C:419:THR:HG21  | 2.35                     | 0.56              |
| 2:C:498:GLN:HA   | 2:C:533:ASP:OD2   | 2.05                     | 0.56              |
| 2:C:715:THR:HB   | 2:C:718:GLY:O     | 2.04                     | 0.56              |
| 3:D:1066:THR:HB  | 3:D:1069:GLU:HG3  | 1.86                     | 0.56              |
| 3:D:1263:PHE:CE1 | 3:D:1352:ILE:HD13 | 2.40                     | 0.56              |
| 3:D:1397:LYS:HB2 | 3:D:1398:TRP:HZ3  | 1.68                     | 0.56              |
| 3:D:1479:ASP:HA  | 3:D:1482:ARG:NE   | 2.19                     | 0.56              |
| 3:D:225:LEU:O    | 3:D:330:THR:HA    | 2.05                     | 0.56              |
| 3:D:249:TYR:HD2  | 3:D:288:MET:HE1   | 1.71                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:40:LEU:HD13   | 4:E:72:ARG:NH1    | 2.20                     | 0.56              |
| 4:E:62:THR:O      | 4:E:66:LYS:HG2    | 2.05                     | 0.56              |
| 5:F:156:VAL:HG23  | 5:F:157:GLU:CD    | 2.26                     | 0.56              |
| 2:M:551:GLU:N     | 2:M:551:GLU:OE1   | 2.39                     | 0.56              |
| 2:M:959:PRO:HA    | 2:M:962:GLN:OE1   | 2.04                     | 0.56              |
| 3:N:1403:LEU:O    | 3:N:1408:ILE:HG13 | 2.05                     | 0.56              |
| 3:N:173:PRO:HG3   | 3:N:209:ARG:HH12  | 1.71                     | 0.56              |
| 3:N:206:ARG:HG3   | 3:N:207:PHE:H     | 1.70                     | 0.56              |
| 2:M:1039:ALA:HB3  | 3:N:713:ILE:HD12  | 1.87                     | 0.56              |
| 3:N:792:ILE:HG21  | 3:N:941:PHE:CD1   | 2.41                     | 0.56              |
| 5:P:172:ARG:HG3   | 5:P:173:TYR:N     | 2.19                     | 0.56              |
| 5:P:300:ASP:CG    | 5:P:302:LYS:HE3   | 2.26                     | 0.56              |
| 5:P:361:LEU:HD12  | 5:P:362:SER:H     | 1.70                     | 0.56              |
| 5:P:370:LYS:HG3   | 5:P:371:LEU:H     | 1.68                     | 0.56              |
| 1:B:47:SER:O      | 1:B:48:ILE:HD12   | 2.05                     | 0.56              |
| 1:B:73:GLU:HG3    | 1:B:130:ALA:HB1   | 1.87                     | 0.56              |
| 2:C:167:LYS:HB3   | 2:C:167:LYS:NZ    | 2.20                     | 0.56              |
| 2:C:198:ARG:HH21  | 2:C:231:PRO:HD3   | 1.70                     | 0.56              |
| 2:C:258:TYR:O     | 2:C:290:LEU:HD12  | 2.05                     | 0.56              |
| 2:C:51:THR:HG21   | 2:C:348:LEU:HG    | 1.87                     | 0.56              |
| 2:C:614:ARG:HA    | 2:C:619:ARG:O     | 2.06                     | 0.56              |
| 2:C:594:ALA:HB1   | 2:C:654:LEU:CD1   | 2.35                     | 0.56              |
| 2:C:672:VAL:HG21  | 2:C:868:ASP:HB2   | 1.87                     | 0.56              |
| 3:D:1149:LEU:HD23 | 3:D:1161:GLU:O    | 2.05                     | 0.56              |
| 3:D:135:LEU:HD11  | 3:D:148:GLU:CG    | 2.36                     | 0.56              |
| 3:D:210:ARG:H     | 3:D:389:GLU:HB2   | 1.70                     | 0.56              |
| 3:D:256:GLU:O     | 3:D:274:ARG:HB2   | 2.04                     | 0.56              |
| 3:D:9:ARG:HG2     | 3:D:10:ILE:N      | 2.20                     | 0.56              |
| 5:F:117:SER:O     | 5:F:121:GLY:N     | 2.38                     | 0.56              |
| 5:F:302:LYS:O     | 5:F:305:GLU:HB3   | 2.05                     | 0.56              |
| 1:K:12:THR:HA     | 1:L:229:GLN:CB    | 2.20                     | 0.56              |
| 1:K:13:VAL:HG22   | 1:K:14:ARG:N      | 2.21                     | 0.56              |
| 2:M:1055:LEU:HD21 | 2:M:1079:PRO:HG3  | 1.87                     | 0.56              |
| 2:M:548:PRO:HG3   | 2:M:842:ARG:NH2   | 2.20                     | 0.56              |
| 2:M:649:VAL:HG13  | 2:M:650:ARG:HH21  | 1.69                     | 0.56              |
| 2:M:7:GLY:HA3     | 2:M:907:ASP:OD2   | 2.05                     | 0.56              |
| 3:N:1041:LEU:HG   | 3:N:1043:GLY:H    | 1.71                     | 0.56              |
| 3:N:1165:TYR:CE2  | 3:N:1214:PRO:HB3  | 2.41                     | 0.56              |
| 3:N:122:GLU:O     | 3:N:126:VAL:CB    | 2.53                     | 0.56              |
| 3:N:169:TYR:HB3   | 3:N:195:VAL:HG11  | 1.88                     | 0.56              |
| 3:N:138:LYS:O     | 3:N:452:ILE:HG22  | 2.06                     | 0.56              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:571:LYS:O    | 3:N:574:LEU:HB3  | 2.06                     | 0.56              |
| 3:N:880:ILE:O    | 3:N:883:ALA:HB3  | 2.05                     | 0.56              |
| 5:P:76:SER:C     | 5:P:78:SER:H     | 2.06                     | 0.56              |
| 1:B:88:ARG:O     | 1:B:120:VAL:HA   | 2.06                     | 0.56              |
| 1:B:85:LEU:HD12  | 1:B:86:VAL:N     | 2.20                     | 0.56              |
| 2:C:1007:ALA:HB2 | 3:D:648:MET:HG3  | 1.88                     | 0.56              |
| 2:C:93:PRO:HA    | 2:C:117:HIS:CA   | 2.35                     | 0.56              |
| 2:C:194:VAL:HA   | 2:C:197:LEU:CD1  | 2.36                     | 0.56              |
| 2:C:405:ARG:NH2  | 2:C:409:ARG:HD2  | 2.21                     | 0.56              |
| 2:C:41:ASN:HB3   | 2:C:49:ARG:CZ    | 2.35                     | 0.56              |
| 2:C:658:GLY:N    | 2:C:661:SER:OG   | 2.39                     | 0.56              |
| 2:C:911:GLU:HB2  | 2:C:912:PRO:HD3  | 1.87                     | 0.56              |
| 3:D:118:LEU:HA   | 3:D:123:LEU:CD1  | 2.32                     | 0.56              |
| 3:D:100:ALA:HB3  | 3:D:128:TYR:HE2  | 1.68                     | 0.56              |
| 3:D:134:VAL:HG12 | 3:D:152:LEU:HA   | 1.86                     | 0.56              |
| 3:D:1365:ASP:O   | 3:D:1366:LYS:C   | 2.44                     | 0.56              |
| 3:D:417:PRO:HB2  | 3:D:428:LYS:CG   | 2.30                     | 0.56              |
| 3:D:545:ARG:HB3  | 3:D:545:ARG:NH1  | 2.19                     | 0.56              |
| 3:D:710:ARG:HG3  | 3:D:711:LEU:HD12 | 1.88                     | 0.56              |
| 5:F:267:THR:HA   | 5:F:270:LYS:HB3  | 1.88                     | 0.56              |
| 5:F:291:ILE:HD12 | 5:F:291:ILE:O    | 2.05                     | 0.56              |
| 2:C:1015:LEU:N   | 5:F:333:ILE:O    | 2.31                     | 0.56              |
| 1:K:71:VAL:HG22  | 1:K:132:LEU:HD22 | 1.87                     | 0.56              |
| 1:L:57:TYR:HB2   | 1:L:164:ALA:HA   | 1.88                     | 0.56              |
| 1:L:99:LEU:HB3   | 1:L:114:PHE:CD2  | 2.41                     | 0.56              |
| 2:M:769:PRO:HG2  | 3:N:65:ARG:HH12  | 1.69                     | 0.56              |
| 3:N:1216:SER:HB2 | 4:O:15:SER:HA    | 1.86                     | 0.56              |
| 3:N:1394:VAL:O   | 3:N:1398:TRP:CD1 | 2.58                     | 0.56              |
| 3:N:1409:ALA:C   | 3:N:1411:GLY:H   | 2.08                     | 0.56              |
| 3:N:135:LEU:HG   | 3:N:151:GLN:O    | 2.04                     | 0.56              |
| 3:N:227:LEU:HD11 | 3:N:327:GLU:N    | 2.20                     | 0.56              |
| 3:N:295:GLY:CA   | 3:N:302:GLN:HB3  | 2.33                     | 0.56              |
| 3:N:511:TRP:N    | 3:N:511:TRP:CE3  | 2.73                     | 0.56              |
| 3:N:598:ARG:HH11 | 3:N:598:ARG:HG2  | 1.71                     | 0.56              |
| 5:P:157:GLU:O    | 5:P:158:GLU:C    | 2.42                     | 0.56              |
| 5:P:305:GLU:HA   | 5:P:308:LEU:HD11 | 1.87                     | 0.56              |
| 1:A:38:ASN:HB3   | 1:A:39:PRO:CD    | 2.32                     | 0.56              |
| 1:B:233:VAL:HG12 | 1:B:235:ALA:H    | 1.70                     | 0.56              |
| 2:C:492:ASP:HA   | 2:C:518:LYS:CB   | 2.35                     | 0.56              |
| 2:C:691:SER:HA   | 2:C:858:MET:CE   | 2.36                     | 0.56              |
| 3:D:403:PHE:CD2  | 3:D:442:ASN:O    | 2.59                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:417:PRO:CB    | 3:D:430:ASP:HA    | 2.32                     | 0.56              |
| 3:D:45:PHE:HB3    | 3:D:86:ARG:HH22   | 1.71                     | 0.56              |
| 3:D:661:MET:C     | 3:D:667:ALA:HB3   | 2.25                     | 0.56              |
| 5:F:321:ILE:HG22  | 5:F:322:GLY:H     | 1.70                     | 0.56              |
| 5:F:343:ASP:N     | 5:F:343:ASP:OD1   | 2.37                     | 0.56              |
| 2:M:203:ASP:HA    | 2:M:228:ALA:HB1   | 1.87                     | 0.56              |
| 2:M:269:LEU:HA    | 2:M:288:ARG:HB2   | 1.88                     | 0.56              |
| 2:M:690:ILE:CG2   | 2:M:852:ILE:HG23  | 2.30                     | 0.56              |
| 3:N:1032:PRO:HB2  | 3:N:1033:GLN:HE22 | 1.71                     | 0.56              |
| 3:N:996:TRP:CD2   | 3:N:1056:PRO:HG2  | 2.41                     | 0.56              |
| 3:N:553:ARG:O     | 3:N:556:LYS:HB2   | 2.05                     | 0.56              |
| 3:N:785:ILE:HG12  | 3:N:939:PHE:CE2   | 2.41                     | 0.56              |
| 3:N:907:GLU:O     | 3:N:908:LYS:C     | 2.44                     | 0.56              |
| 5:P:278:LEU:CB    | 5:P:286:PRO:HG3   | 2.24                     | 0.56              |
| 5:P:411:HIS:O     | 5:P:414:ARG:HB2   | 2.05                     | 0.56              |
| 1:B:176:ARG:HD3   | 3:D:884:ARG:HH22  | 1.70                     | 0.56              |
| 1:B:38:ASN:CB     | 1:B:39:PRO:HD3    | 2.32                     | 0.56              |
| 2:C:198:ARG:HG3   | 2:C:231:PRO:HA    | 1.86                     | 0.56              |
| 2:C:408:ARG:NH2   | 2:C:457:ALA:O     | 2.38                     | 0.56              |
| 2:C:44:ILE:O      | 2:C:47:ALA:HB3    | 2.06                     | 0.56              |
| 3:D:210:ARG:HB2   | 3:D:389:GLU:CB    | 2.35                     | 0.56              |
| 3:D:280:ALA:HB1   | 3:D:282:TYR:CZ    | 2.40                     | 0.56              |
| 3:D:403:PHE:CE1   | 3:D:442:ASN:HB3   | 2.41                     | 0.56              |
| 3:D:596:SER:C     | 3:D:598:ARG:H     | 2.09                     | 0.56              |
| 4:E:28:GLN:O      | 4:E:31:LEU:HB2    | 2.05                     | 0.56              |
| 5:F:131:VAL:O     | 5:F:135:ILE:HG13  | 2.05                     | 0.56              |
| 5:F:264:MET:HE2   | 5:F:264:MET:HA    | 1.88                     | 0.56              |
| 5:F:368:VAL:HG23  | 5:F:369:LEU:HG    | 1.88                     | 0.56              |
| 5:F:418:LEU:H     | 5:F:418:LEU:CD1   | 2.02                     | 0.56              |
| 1:K:13:VAL:CG2    | 1:K:14:ARG:N      | 2.68                     | 0.56              |
| 1:L:68:ILE:HD12   | 1:L:71:VAL:HG11   | 1.86                     | 0.56              |
| 1:L:97:VAL:HG12   | 1:L:98:THR:N      | 2.21                     | 0.56              |
| 2:M:1030:GLN:HE22 | 3:N:628:ARG:HH21  | 1.53                     | 0.56              |
| 2:M:400:PRO:O     | 2:M:401:LEU:C     | 2.42                     | 0.56              |
| 2:M:710:ILE:CG2   | 2:M:823:VAL:HB    | 2.36                     | 0.56              |
| 3:N:207:PHE:HB2   | 3:N:391:ALA:HB3   | 1.87                     | 0.56              |
| 3:N:219:GLU:C     | 3:N:337:LEU:HG    | 2.26                     | 0.56              |
| 3:N:23:TYR:O      | 3:N:49:ILE:HG23   | 2.06                     | 0.56              |
| 3:N:284:LEU:HD13  | 3:N:288:MET:CG    | 2.34                     | 0.56              |
| 3:N:536:ALA:O     | 3:N:537:THR:HG23  | 2.06                     | 0.56              |
| 3:N:602:SER:O     | 3:N:606:ILE:HG13  | 2.06                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:O:6:ILE:HA      | 4:O:9:LEU:HD12    | 1.88                     | 0.56              |
| 1:A:209:GLU:HA    | 1:A:212:ASN:HD22  | 1.71                     | 0.56              |
| 1:A:5:LYS:NZ      | 1:A:28:LEU:C      | 2.59                     | 0.56              |
| 1:B:19:GLU:HG2    | 1:B:203:GLY:CA    | 2.35                     | 0.56              |
| 2:C:164:PRO:HB3   | 2:C:264:PRO:O     | 2.05                     | 0.56              |
| 2:C:198:ARG:HE    | 2:C:231:PRO:CD    | 2.19                     | 0.56              |
| 2:C:649:VAL:HA    | 2:C:650:ARG:NH2   | 2.17                     | 0.56              |
| 2:C:807:ARG:CZ    | 2:C:807:ARG:HB2   | 2.35                     | 0.56              |
| 3:D:1161:GLU:HG3  | 3:D:1164:ARG:CB   | 2.29                     | 0.56              |
| 3:D:540:LEU:HD21  | 3:D:606:ILE:CD1   | 2.36                     | 0.56              |
| 3:D:794:GLN:NE2   | 3:D:905:PRO:HG2   | 2.19                     | 0.56              |
| 5:F:159:ILE:O     | 5:F:163:LEU:HG    | 2.06                     | 0.56              |
| 5:F:402:ASN:HD22  | 5:F:402:ASN:N     | 2.04                     | 0.56              |
| 5:F:402:ASN:H     | 5:F:402:ASN:ND2   | 2.03                     | 0.56              |
| 1:L:112:ARG:HH11  | 1:L:112:ARG:HB3   | 1.70                     | 0.56              |
| 1:L:86:VAL:CG1    | 1:L:123:MET:HB2   | 2.36                     | 0.56              |
| 2:M:204:GLN:HB2   | 2:M:209:ARG:CZ    | 2.36                     | 0.56              |
| 2:M:31:GLN:HG2    | 2:M:35:PRO:CB     | 2.31                     | 0.56              |
| 2:M:72:ARG:O      | 2:M:95:TYR:N      | 2.38                     | 0.56              |
| 3:N:1094:LEU:HD12 | 3:N:1098:LEU:HD11 | 1.87                     | 0.56              |
| 3:N:1365:ASP:O    | 3:N:1366:LYS:C    | 2.44                     | 0.56              |
| 3:N:592:THR:CG2   | 3:N:600:LEU:HD21  | 2.31                     | 0.56              |
| 3:N:69:GLU:HG3    | 3:N:71:LYS:HZ3    | 1.70                     | 0.56              |
| 3:N:965:GLU:O     | 3:N:966:GLU:C     | 2.44                     | 0.56              |
| 5:P:231:ARG:HB2   | 5:P:233:PHE:CZ    | 2.41                     | 0.56              |
| 5:P:270:LYS:HA    | 5:P:273:ARG:HD2   | 1.87                     | 0.56              |
| 5:P:84:TYR:O      | 5:P:86:HIS:N      | 2.39                     | 0.56              |
| 2:C:230:ARG:HH11  | 2:C:230:ARG:HG3   | 1.71                     | 0.56              |
| 2:C:380:ALA:O     | 2:C:381:ALA:C     | 2.42                     | 0.56              |
| 2:C:439:CYS:SG    | 2:C:441:VAL:HG13  | 2.46                     | 0.56              |
| 2:C:460:ARG:HH21  | 2:C:462:ASP:HB3   | 1.70                     | 0.56              |
| 3:D:1156:LEU:HD12 | 3:D:1173:LEU:CD1  | 2.35                     | 0.56              |
| 3:D:1310:ARG:HB3  | 3:D:1327:ARG:HG3  | 1.88                     | 0.56              |
| 3:D:1344:VAL:CG1  | 3:D:1345:GLU:N    | 2.69                     | 0.56              |
| 3:D:1440:PHE:HE2  | 3:D:1463:LYS:NZ   | 2.03                     | 0.56              |
| 3:D:520:LEU:O     | 3:D:525:ARG:NH1   | 2.39                     | 0.56              |
| 3:D:685:ASP:O     | 3:D:687:VAL:N     | 2.39                     | 0.56              |
| 3:D:71:LYS:H      | 3:D:80:VAL:CG2    | 2.19                     | 0.56              |
| 3:D:959:GLU:CD    | 3:D:959:GLU:H     | 2.09                     | 0.56              |
| 5:F:223:ALA:HB2   | 5:F:242:TRP:CG    | 2.41                     | 0.56              |
| 5:F:244:ARG:O     | 5:F:247:ILE:HB    | 2.06                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:271:LEU:O    | 5:F:272:SER:C     | 2.44                     | 0.56              |
| 1:K:111:ALA:HB3  | 1:K:124:ASN:O     | 2.05                     | 0.56              |
| 2:M:358:ARG:HD2  | 2:M:372:LEU:HA    | 1.86                     | 0.56              |
| 2:M:486:MET:SD   | 2:M:491:GLU:HA    | 2.46                     | 0.56              |
| 2:M:545:ASN:CB   | 2:M:583:LEU:HD11  | 2.35                     | 0.56              |
| 2:M:600:ASP:HB3  | 2:M:650:ARG:CA    | 2.29                     | 0.56              |
| 3:N:1216:SER:OG  | 4:O:16:LYS:HB2    | 2.05                     | 0.56              |
| 3:N:152:LEU:HG   | 3:N:153:LEU:N     | 2.19                     | 0.56              |
| 3:N:188:GLY:N    | 3:N:197:SER:O     | 2.39                     | 0.56              |
| 3:N:470:LEU:N    | 3:N:470:LEU:HD23  | 2.20                     | 0.56              |
| 1:A:44:LEU:O     | 1:A:48:ILE:HG12   | 2.06                     | 0.56              |
| 1:B:188:GLN:HG2  | 1:B:189:ARG:HG3   | 1.88                     | 0.56              |
| 1:B:76:VAL:HA    | 1:B:79:ILE:CG1    | 2.36                     | 0.56              |
| 2:C:1008:ARG:HG2 | 2:C:1009:SER:N    | 2.21                     | 0.56              |
| 2:C:691:SER:HA   | 2:C:858:MET:HE3   | 1.88                     | 0.56              |
| 2:C:876:VAL:O    | 2:C:880:MET:N     | 2.39                     | 0.56              |
| 2:C:950:LEU:HB2  | 2:C:952:LEU:HG    | 1.87                     | 0.56              |
| 3:D:758:GLU:HG2  | 3:D:1476:THR:HG21 | 1.88                     | 0.56              |
| 3:D:442:ASN:ND2  | 3:D:442:ASN:N     | 2.54                     | 0.56              |
| 3:D:583:ASP:HB2  | 3:D:604:THR:OG1   | 2.05                     | 0.56              |
| 2:C:1031:ARG:HB2 | 3:D:622:ARG:HH12  | 1.71                     | 0.56              |
| 3:D:821:VAL:HG22 | 3:D:840:LYS:NZ    | 2.21                     | 0.56              |
| 3:D:937:TYR:HA   | 3:D:940:THR:OG1   | 2.06                     | 0.56              |
| 4:E:45:ARG:O     | 4:E:47:LYS:HG2    | 2.06                     | 0.56              |
| 5:F:142:ARG:CD   | 5:F:145:PRO:HA    | 2.35                     | 0.56              |
| 1:K:208:LEU:O    | 1:K:211:LEU:HB3   | 2.05                     | 0.56              |
| 1:L:179:PHE:CB   | 1:L:197:LEU:HD13  | 2.34                     | 0.56              |
| 2:M:1083:GLU:O   | 2:M:1087:VAL:HG23 | 2.05                     | 0.56              |
| 2:M:328:LEU:HD11 | 2:M:434:HIS:HA    | 1.87                     | 0.56              |
| 2:M:115:LEU:HB3  | 2:M:375:SER:HB3   | 1.88                     | 0.56              |
| 3:N:1048:PRO:HA  | 3:N:1079:LYS:NZ   | 2.20                     | 0.56              |
| 3:N:225:LEU:HD11 | 3:N:242:LEU:HD21  | 1.88                     | 0.56              |
| 3:N:420:VAL:C    | 3:N:421:LEU:HD23  | 2.26                     | 0.56              |
| 3:N:566:ILE:O    | 3:N:569:ASN:HB3   | 2.05                     | 0.56              |
| 3:N:574:LEU:HG   | 3:N:575:GLN:N     | 2.20                     | 0.56              |
| 3:N:925:GLU:HG2  | 4:O:7:ASP:OD2     | 2.05                     | 0.56              |
| 1:A:85:LEU:HD12  | 1:A:124:ASN:OD1   | 2.05                     | 0.55              |
| 2:C:1005:MET:HG2 | 3:D:629:SER:CB    | 2.35                     | 0.55              |
| 2:C:305:PRO:HG3  | 2:C:308:ARG:NH2   | 2.20                     | 0.55              |
| 2:C:522:VAL:HG12 | 2:C:523:ILE:N     | 2.20                     | 0.55              |
| 3:D:102:ILE:O    | 3:D:104:PHE:N     | 2.39                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:102:ILE:C     | 3:D:104:PHE:H    | 2.10                     | 0.55              |
| 3:D:119:SER:CB    | 3:D:123:LEU:H    | 2.02                     | 0.55              |
| 3:D:1280:VAL:HG12 | 3:D:1281:VAL:N   | 2.21                     | 0.55              |
| 3:D:1465:ASN:HD22 | 3:D:1473:PRO:HD3 | 1.69                     | 0.55              |
| 3:D:248:PRO:CB    | 3:D:308:LYS:NZ   | 2.69                     | 0.55              |
| 3:D:406:ASP:CB    | 3:D:424:GLY:H    | 2.18                     | 0.55              |
| 3:D:398:ALA:HB2   | 3:D:447:VAL:HG22 | 1.88                     | 0.55              |
| 3:D:5:VAL:HG22    | 3:D:6:ARG:H      | 1.71                     | 0.55              |
| 3:D:72:VAL:HG12   | 3:D:73:CYS:N     | 2.21                     | 0.55              |
| 3:D:864:VAL:CG1   | 3:D:865:THR:N    | 2.69                     | 0.55              |
| 3:D:957:PRO:HG3   | 3:D:1010:ASN:ND2 | 2.04                     | 0.55              |
| 4:E:6:ILE:CG2     | 4:E:7:ASP:N      | 2.69                     | 0.55              |
| 5:F:386:VAL:CG2   | 5:F:387:GLY:N    | 2.69                     | 0.55              |
| 2:M:191:PHE:CD2   | 2:M:195:LEU:HD12 | 2.42                     | 0.55              |
| 2:M:879:ARG:HD2   | 2:M:879:ARG:N    | 2.21                     | 0.55              |
| 2:M:974:LEU:HD11  | 2:M:989:VAL:HG11 | 1.87                     | 0.55              |
| 3:N:1194:CYS:HB2  | 3:N:1204:CYS:CB  | 2.36                     | 0.55              |
| 3:N:246:PRO:HD2   | 3:N:308:LYS:HA   | 1.88                     | 0.55              |
| 5:P:365:GLU:HA    | 5:P:368:VAL:HG13 | 1.88                     | 0.55              |
| 1:A:1:MET:HA      | 1:A:6:LEU:HD22   | 1.88                     | 0.55              |
| 2:C:355:VAL:HA    | 2:C:358:ARG:HG3  | 1.89                     | 0.55              |
| 2:C:415:PRO:HG2   | 2:C:418:LEU:HD12 | 1.88                     | 0.55              |
| 2:C:56:GLU:OE1    | 2:C:359:MET:HB2  | 2.05                     | 0.55              |
| 2:C:768:THR:HB    | 2:C:771:GLU:HB3  | 1.88                     | 0.55              |
| 1:A:30:ARG:HG3    | 2:C:938:LYS:NZ   | 2.22                     | 0.55              |
| 2:C:939:ARG:O     | 2:C:942:GLU:HB3  | 2.05                     | 0.55              |
| 3:D:1094:LEU:HG   | 3:D:1095:THR:N   | 2.21                     | 0.55              |
| 3:D:1293:PHE:CE2  | 3:D:1300:SER:HB3 | 2.41                     | 0.55              |
| 3:D:136:ASP:HB2   | 3:D:453:ASP:O    | 2.05                     | 0.55              |
| 3:D:884:ARG:HG2   | 3:D:885:ILE:N    | 2.21                     | 0.55              |
| 5:F:162:LYS:O     | 5:F:166:LEU:HG   | 2.07                     | 0.55              |
| 5:F:221:ILE:O     | 5:F:224:VAL:HB   | 2.06                     | 0.55              |
| 5:F:401:GLU:O     | 5:F:404:ALA:HB3  | 2.06                     | 0.55              |
| 2:M:98:LEU:H      | 2:M:111:ASP:HA   | 1.71                     | 0.55              |
| 2:M:224:GLU:HB3   | 2:M:227:PHE:CB   | 2.36                     | 0.55              |
| 2:M:277:ALA:O     | 2:M:281:LEU:N    | 2.39                     | 0.55              |
| 2:M:498:GLN:HB2   | 2:M:514:VAL:CG2  | 2.36                     | 0.55              |
| 2:M:573:ARG:O     | 2:M:670:GLN:NE2  | 2.39                     | 0.55              |
| 2:M:89:THR:HG23   | 2:M:128:ILE:O    | 2.06                     | 0.55              |
| 3:N:1253:THR:HG22 | 3:N:1254:GLN:N   | 2.18                     | 0.55              |
| 3:N:413:ASP:O     | 3:N:434:ARG:HA   | 2.06                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:5:VAL:HG12    | 3:N:6:ARG:N       | 2.22                     | 0.55              |
| 3:N:857:ILE:O     | 3:N:858:VAL:HG23  | 2.05                     | 0.55              |
| 3:N:350:HIS:HB3   | 5:P:232:ARG:CZ    | 2.36                     | 0.55              |
| 5:P:262:VAL:HA    | 5:P:265:VAL:HG23  | 1.88                     | 0.55              |
| 5:P:399:GLN:O     | 5:P:402:ASN:HB2   | 2.06                     | 0.55              |
| 5:P:86:HIS:C      | 5:P:88:ILE:N      | 2.60                     | 0.55              |
| 1:B:58:ILE:CD1    | 1:B:60:ASP:H      | 2.19                     | 0.55              |
| 2:C:1015:LEU:HA   | 5:F:335:ASP:HB2   | 1.88                     | 0.55              |
| 2:C:948:GLU:HB3   | 2:C:953:VAL:HG23  | 1.88                     | 0.55              |
| 3:D:10:ILE:O      | 3:D:10:ILE:HG23   | 2.06                     | 0.55              |
| 3:D:1246:VAL:CG1  | 3:D:1249:ALA:O    | 2.54                     | 0.55              |
| 3:D:1504:GLU:O    | 3:D:1505:ALA:HB3  | 2.05                     | 0.55              |
| 3:D:245:LEU:HG    | 3:D:309:GLY:HA2   | 1.88                     | 0.55              |
| 3:D:41:ARG:HH21   | 3:D:48:ARG:NH1    | 2.03                     | 0.55              |
| 3:D:810:GLU:O     | 3:D:812:ALA:N     | 2.40                     | 0.55              |
| 3:D:828:LYS:N     | 3:D:828:LYS:HD3   | 2.21                     | 0.55              |
| 3:D:984:THR:HG23  | 3:D:987:GLU:H     | 1.72                     | 0.55              |
| 3:D:1481:VAL:HG22 | 4:E:18:ARG:CZ     | 2.36                     | 0.55              |
| 5:F:94:LEU:HD11   | 5:F:190:ALA:CB    | 2.36                     | 0.55              |
| 2:C:1015:LEU:HB2  | 5:F:333:ILE:HG22  | 1.88                     | 0.55              |
| 1:K:42:ARG:HD3    | 1:L:35:THR:HA     | 1.89                     | 0.55              |
| 1:L:210:ALA:O     | 1:L:211:LEU:C     | 2.45                     | 0.55              |
| 2:M:560:MET:HB3   | 2:M:564:MET:CE    | 2.37                     | 0.55              |
| 3:N:1302:GLU:HG2  | 3:N:1303:TYR:N    | 2.20                     | 0.55              |
| 3:N:1311:LEU:CD1  | 3:N:1312:LEU:H    | 2.17                     | 0.55              |
| 3:N:1363:LEU:C    | 3:N:1363:LEU:HD23 | 2.27                     | 0.55              |
| 3:N:1377:LYS:HD3  | 3:N:1378:TYR:CE1  | 2.41                     | 0.55              |
| 3:N:167:GLU:OE1   | 3:N:169:TYR:CE2   | 2.60                     | 0.55              |
| 3:N:591:VAL:HG12  | 3:N:599:PRO:CA    | 2.36                     | 0.55              |
| 3:N:875:THR:HG21  | 3:N:902:LEU:HD11  | 1.87                     | 0.55              |
| 5:P:305:GLU:OE2   | 5:P:309:LYS:NZ    | 2.37                     | 0.55              |
| 5:P:321:ILE:O     | 5:P:323:ASP:N     | 2.40                     | 0.55              |
| 1:A:83:LYS:HZ1    | 1:A:170:VAL:HG22  | 1.71                     | 0.55              |
| 2:C:373:VAL:CG1   | 2:C:374:ASN:N     | 2.69                     | 0.55              |
| 3:D:1353:GLN:O    | 3:D:1355:VAL:N    | 2.39                     | 0.55              |
| 3:D:166:GLN:HB3   | 3:D:394:LEU:HD11  | 1.89                     | 0.55              |
| 3:D:16:GLU:N      | 3:D:16:GLU:CD     | 2.57                     | 0.55              |
| 3:D:274:ARG:HE    | 3:D:279:VAL:HG11  | 1.71                     | 0.55              |
| 3:D:296:GLU:N     | 3:D:302:GLN:OE1   | 2.39                     | 0.55              |
| 3:D:41:ARG:HH11   | 3:D:41:ARG:HG3    | 1.70                     | 0.55              |
| 3:D:629:SER:HB3   | 3:D:726:ILE:HD11  | 1.89                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:175:HIS:HA    | 5:F:178:ARG:HB2   | 1.87                     | 0.55              |
| 5:F:373:LYS:HB3   | 5:F:379:ARG:H     | 1.70                     | 0.55              |
| 1:L:79:ILE:HA     | 1:L:82:LEU:HG     | 1.88                     | 0.55              |
| 2:M:953:VAL:HG13  | 2:M:966:LEU:HD13  | 1.88                     | 0.55              |
| 3:N:1337:GLU:CD   | 3:N:1337:GLU:H    | 2.09                     | 0.55              |
| 3:N:191:LEU:HD23  | 3:N:195:VAL:HG11  | 1.88                     | 0.55              |
| 3:N:41:ARG:HH21   | 3:N:48:ARG:NH1    | 2.04                     | 0.55              |
| 3:N:522:PRO:HG3   | 3:N:525:ARG:HH22  | 1.70                     | 0.55              |
| 3:N:544:TYR:O     | 3:N:545:ARG:C     | 2.42                     | 0.55              |
| 5:P:147:LEU:O     | 5:P:148:LYS:HB2   | 2.05                     | 0.55              |
| 1:B:176:ARG:HG2   | 1:B:177:VAL:H     | 1.71                     | 0.55              |
| 1:B:63:HIS:HD2    | 1:B:65:PHE:HB2    | 1.71                     | 0.55              |
| 1:B:68:ILE:HD12   | 1:B:71:VAL:CG1    | 2.37                     | 0.55              |
| 2:C:1066:ALA:O    | 2:C:1070:ILE:HG13 | 2.06                     | 0.55              |
| 2:C:1114:GLY:C    | 2:C:1116:ALA:H    | 2.09                     | 0.55              |
| 2:C:23:VAL:HG23   | 2:C:24:GLU:N      | 2.21                     | 0.55              |
| 2:C:266:ARG:CD    | 2:C:273:GLY:HA3   | 2.37                     | 0.55              |
| 2:C:493:ARG:HB2   | 2:C:494:TYR:CE1   | 2.42                     | 0.55              |
| 3:D:1028:ALA:O    | 3:D:1029:ARG:HB2  | 2.06                     | 0.55              |
| 3:D:1376:MET:HE1  | 3:D:1421:LEU:CD1  | 2.37                     | 0.55              |
| 3:D:28:LYS:HG2    | 3:D:42:ASP:CB     | 2.36                     | 0.55              |
| 3:D:128:TYR:CD1   | 3:D:457:GLY:HA2   | 2.27                     | 0.55              |
| 3:D:529:GLN:HA    | 3:D:535:PHE:CD2   | 2.40                     | 0.55              |
| 3:D:654:LYS:O     | 3:D:658:LEU:HG    | 2.07                     | 0.55              |
| 3:D:409:VAL:HB    | 5:F:164:LYS:NZ    | 2.22                     | 0.55              |
| 1:K:55:SER:HA     | 1:K:167:VAL:HG23  | 1.88                     | 0.55              |
| 1:K:74:ASP:OD1    | 1:K:76:VAL:N      | 2.39                     | 0.55              |
| 1:L:74:ASP:OD2    | 1:L:75:VAL:N      | 2.40                     | 0.55              |
| 2:M:1059:ASP:HA   | 2:M:1083:GLU:OE2  | 2.07                     | 0.55              |
| 2:M:1111:ILE:HD11 | 2:M:1112:PHE:CE1  | 2.41                     | 0.55              |
| 2:M:641:PRO:HA    | 2:M:655:LEU:O     | 2.06                     | 0.55              |
| 3:N:1126:ASP:OD2  | 3:N:1129:THR:HG23 | 2.06                     | 0.55              |
| 3:N:1304:LYS:O    | 3:N:1305:LEU:HB3  | 2.05                     | 0.55              |
| 3:N:36:THR:CG2    | 3:N:38:LYS:HE2    | 2.37                     | 0.55              |
| 3:N:622:ARG:HG2   | 3:N:622:ARG:HH11  | 1.72                     | 0.55              |
| 3:N:835:SER:HB3   | 3:N:838:ARG:HG3   | 1.89                     | 0.55              |
| 3:N:891:GLU:HB2   | 3:N:926:LYS:NZ    | 2.21                     | 0.55              |
| 5:P:209:PHE:HA    | 5:P:212:LEU:CD1   | 2.36                     | 0.55              |
| 5:P:406:ARG:O     | 5:P:409:LYS:HG3   | 2.06                     | 0.55              |
| 1:A:206:THR:HG22  | 1:A:208:LEU:H     | 1.70                     | 0.55              |
| 1:B:112:ARG:O     | 1:B:114:PHE:N     | 2.40                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:34:VAL:CB     | 1:B:42:ARG:HH12   | 1.96                     | 0.55              |
| 2:C:95:TYR:CG     | 2:C:114:PHE:HB3   | 2.41                     | 0.55              |
| 2:C:32:ALA:C      | 2:C:35:PRO:HD2    | 2.27                     | 0.55              |
| 2:C:806:LEU:HD22  | 2:C:813:VAL:CG2   | 2.36                     | 0.55              |
| 3:D:1103:HIS:CD2  | 3:D:1462:LEU:H    | 2.24                     | 0.55              |
| 3:D:119:SER:OG    | 3:D:122:GLU:HB2   | 2.07                     | 0.55              |
| 3:D:1398:TRP:HB3  | 3:D:1402:ALA:HB3  | 1.89                     | 0.55              |
| 3:D:1409:ALA:C    | 3:D:1410:GLU:HG3  | 2.26                     | 0.55              |
| 3:D:178:LEU:HG    | 3:D:181:ASP:CB    | 2.35                     | 0.55              |
| 3:D:14:SER:O      | 3:D:18:ILE:HG13   | 2.05                     | 0.55              |
| 3:D:288:MET:O     | 3:D:290:PRO:HD3   | 2.05                     | 0.55              |
| 3:D:365:ASP:O     | 3:D:379:ALA:CB    | 2.54                     | 0.55              |
| 3:D:494:LYS:HA    | 3:D:1388:ARG:HH12 | 1.72                     | 0.55              |
| 3:D:508:ARG:CB    | 3:D:510:GLU:OE1   | 2.54                     | 0.55              |
| 3:D:673:ALA:O     | 3:D:677:LEU:HG    | 2.07                     | 0.55              |
| 3:D:826:PRO:HD2   | 3:D:829:VAL:HG11  | 1.89                     | 0.55              |
| 3:D:914:LEU:O     | 3:D:914:LEU:HD12  | 2.07                     | 0.55              |
| 3:D:986:ARG:HG3   | 3:D:990:ASP:OD2   | 2.05                     | 0.55              |
| 4:E:5:GLY:O       | 4:E:9:LEU:HG      | 2.05                     | 0.55              |
| 5:F:127:ILE:O     | 5:F:130:VAL:N     | 2.39                     | 0.55              |
| 5:F:245:GLN:CA    | 5:F:245:GLN:NE2   | 2.70                     | 0.55              |
| 5:F:288:TYR:O     | 5:F:291:ILE:HG23  | 2.06                     | 0.55              |
| 5:F:314:PRO:HG2   | 5:F:315:VAL:N     | 2.21                     | 0.55              |
| 5:F:75:ILE:HG22   | 5:F:76:SER:N      | 2.21                     | 0.55              |
| 5:F:80:PRO:HA     | 5:F:83:GLN:NE2    | 2.16                     | 0.55              |
| 1:K:203:GLY:C     | 1:K:205:VAL:N     | 2.59                     | 0.55              |
| 1:L:28:LEU:HD13   | 1:L:33:GLY:N      | 2.22                     | 0.55              |
| 1:L:32:PHE:O      | 1:L:36:LEU:HD12   | 2.06                     | 0.55              |
| 2:M:1056:LYS:HZ3  | 3:N:749:VAL:H     | 1.54                     | 0.55              |
| 2:M:200:LEU:HD13  | 2:M:300:ASP:HB3   | 1.88                     | 0.55              |
| 2:M:389:SER:HB3   | 2:M:392:SER:HB3   | 1.89                     | 0.55              |
| 2:M:790:LEU:HD12  | 2:M:790:LEU:C     | 2.27                     | 0.55              |
| 2:M:892:LEU:O     | 2:M:895:TYR:HB3   | 2.07                     | 0.55              |
| 3:N:1394:VAL:HG21 | 3:N:1397:LYS:NZ   | 2.22                     | 0.55              |
| 3:N:1492:LEU:O    | 3:N:1495:ILE:HG22 | 2.07                     | 0.55              |
| 3:N:323:GLU:HB2   | 3:N:334:THR:CB    | 2.36                     | 0.55              |
| 3:N:430:ASP:N     | 3:N:430:ASP:OD1   | 2.38                     | 0.55              |
| 3:N:525:ARG:NH1   | 3:N:525:ARG:HG2   | 2.20                     | 0.55              |
| 2:C:139:GLN:HG2   | 2:C:391:LEU:HD21  | 1.87                     | 0.55              |
| 2:C:176:VAL:HG12  | 2:C:183:SER:N     | 2.21                     | 0.55              |
| 2:C:396:ASP:O     | 2:C:403:SER:CA    | 2.54                     | 0.55              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:410:ILE:HD12 | 2:C:410:ILE:N     | 2.22                     | 0.55              |
| 2:C:600:ASP:HA   | 2:C:649:VAL:O     | 2.06                     | 0.55              |
| 2:C:879:ARG:N    | 2:C:879:ARG:HD2   | 2.22                     | 0.55              |
| 2:C:989:VAL:HG23 | 2:C:990:GLY:N     | 2.21                     | 0.55              |
| 3:D:954:ALA:CB   | 3:D:1062:ARG:HD2  | 2.33                     | 0.55              |
| 3:D:108:VAL:HG12 | 3:D:109:PRO:HA    | 1.86                     | 0.55              |
| 3:D:1220:ALA:O   | 3:D:1224:VAL:HG23 | 2.07                     | 0.55              |
| 3:D:1481:VAL:O   | 3:D:1482:ARG:C    | 2.45                     | 0.55              |
| 3:D:573:MET:O    | 3:D:576:GLU:HB3   | 2.06                     | 0.55              |
| 3:D:655:PRO:O    | 3:D:656:PHE:C     | 2.45                     | 0.55              |
| 3:D:864:VAL:CG1  | 3:D:865:THR:H     | 2.20                     | 0.55              |
| 4:E:80:VAL:HB    | 4:E:81:PRO:HD2    | 1.89                     | 0.55              |
| 5:F:117:SER:HB2  | 5:F:122:LEU:O     | 2.06                     | 0.55              |
| 5:F:401:GLU:O    | 5:F:405:LEU:HG    | 2.07                     | 0.55              |
| 1:K:86:VAL:HG12  | 1:K:124:ASN:OD1   | 2.06                     | 0.55              |
| 1:L:10:VAL:HG22  | 1:L:26:GLU:O      | 2.07                     | 0.55              |
| 1:L:28:LEU:HD11  | 1:L:36:LEU:CD1    | 2.37                     | 0.55              |
| 2:M:474:VAL:HG11 | 2:M:529:VAL:HG12  | 1.89                     | 0.55              |
| 2:M:87:ASP:O     | 2:M:130:ASN:HA    | 2.07                     | 0.55              |
| 1:K:198:ARG:NH2  | 2:M:932:GLU:OE2   | 2.40                     | 0.55              |
| 3:N:1012:GLU:HB2 | 3:N:1021:TYR:OH   | 2.07                     | 0.55              |
| 3:N:1211:MET:HB2 | 3:N:1213:ARG:NH1  | 2.21                     | 0.55              |
| 3:N:1404:ASN:CA  | 3:N:1408:ILE:HB   | 2.35                     | 0.55              |
| 3:N:264:LEU:HD22 | 3:N:316:GLN:NE2   | 2.21                     | 0.55              |
| 3:N:317:VAL:HB   | 3:N:339:TRP:HB3   | 1.89                     | 0.55              |
| 3:N:607:LEU:HG   | 3:N:608:SER:N     | 2.21                     | 0.55              |
| 2:M:1030:GLN:OE1 | 3:N:628:ARG:HB2   | 2.06                     | 0.55              |
| 3:N:760:ARG:NH1  | 4:O:61:GLU:HB2    | 2.22                     | 0.55              |
| 3:N:970:LYS:HG3  | 3:N:974:ILE:HD11  | 1.89                     | 0.55              |
| 2:C:437:ARG:O    | 2:C:455:LEU:HD12  | 2.07                     | 0.55              |
| 2:C:560:MET:HB3  | 2:C:564:MET:HE3   | 1.87                     | 0.55              |
| 2:C:815:LEU:CD1  | 2:C:821:GLU:HA    | 2.37                     | 0.55              |
| 3:D:1294:VAL:O   | 3:D:1295:GLU:HG3  | 2.07                     | 0.55              |
| 3:D:1377:LYS:HD3 | 3:D:1378:TYR:CE1  | 2.42                     | 0.55              |
| 3:D:1448:THR:O   | 3:D:1452:ILE:HG12 | 2.07                     | 0.55              |
| 3:D:209:ARG:N    | 3:D:389:GLU:O     | 2.40                     | 0.55              |
| 4:E:6:ILE:CG2    | 4:E:7:ASP:H       | 2.19                     | 0.55              |
| 5:F:138:SER:O    | 5:F:141:VAL:HG22  | 2.07                     | 0.55              |
| 1:L:108:GLU:HG3  | 1:L:131:THR:CG2   | 2.33                     | 0.55              |
| 1:L:66:SER:O     | 1:L:75:VAL:HG23   | 2.07                     | 0.55              |
| 2:M:1006:HIS:HA  | 2:M:1027:PHE:CZ   | 2.41                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:151:ASP:H    | 2:M:158:TYR:HA    | 1.71                     | 0.55              |
| 2:M:235:LEU:HD22 | 2:M:236:ILE:HG13  | 1.89                     | 0.55              |
| 2:M:841:ASN:ND2  | 2:M:884:GLN:OE1   | 2.40                     | 0.55              |
| 3:N:1030:GLY:HA2 | 3:N:1034:GLN:NE2  | 2.22                     | 0.55              |
| 3:N:1221:VAL:CG1 | 3:N:1370:ILE:HD13 | 2.37                     | 0.55              |
| 3:N:139:GLY:O    | 3:N:147:VAL:HB    | 2.06                     | 0.55              |
| 3:N:261:LEU:HD23 | 3:N:270:LEU:HA    | 1.88                     | 0.55              |
| 3:N:218:LYS:HA   | 3:N:337:LEU:O     | 2.07                     | 0.55              |
| 3:N:18:ILE:HG23  | 3:N:518:PRO:HG3   | 1.89                     | 0.55              |
| 3:N:610:LYS:NZ   | 3:N:1442:ASN:N    | 2.52                     | 0.55              |
| 3:N:637:LEU:HD12 | 3:N:729:HIS:N     | 2.21                     | 0.55              |
| 3:N:921:ARG:HH11 | 3:N:921:ARG:CB    | 2.19                     | 0.55              |
| 5:P:128:ARG:HA   | 5:P:131:VAL:CG2   | 2.36                     | 0.55              |
| 5:P:245:GLN:CA   | 5:P:245:GLN:HE21  | 2.20                     | 0.55              |
| 5:P:382:THR:HG23 | 5:P:397:ILE:CG2   | 2.37                     | 0.55              |
| 1:A:86:VAL:HG22  | 1:A:123:MET:HG3   | 1.89                     | 0.55              |
| 2:C:293:PHE:HD1  | 2:C:294:GLU:N     | 2.04                     | 0.55              |
| 2:C:599:GLU:HA   | 2:C:599:GLU:OE1   | 2.07                     | 0.55              |
| 2:C:728:HIS:ND1  | 2:C:729:LEU:N     | 2.55                     | 0.55              |
| 2:C:695:LEU:HD21 | 2:C:833:LEU:HB3   | 1.89                     | 0.55              |
| 3:D:1078:ARG:HG3 | 3:D:1078:ARG:HH11 | 1.72                     | 0.55              |
| 3:D:1104:GLU:O   | 3:D:1106:VAL:HG23 | 2.07                     | 0.55              |
| 3:D:1354:LYS:O   | 3:D:1358:ALA:HB2  | 2.07                     | 0.55              |
| 3:D:178:LEU:HG   | 3:D:181:ASP:OD2   | 2.07                     | 0.55              |
| 3:D:413:ASP:O    | 3:D:434:ARG:HA    | 2.07                     | 0.55              |
| 3:D:133:ILE:HG22 | 3:D:455:ARG:C     | 2.27                     | 0.55              |
| 3:D:99:ALA:N     | 3:D:514:LEU:O     | 2.39                     | 0.55              |
| 3:D:812:ALA:C    | 3:D:814:ALA:N     | 2.59                     | 0.55              |
| 3:D:869:MET:HE1  | 3:D:893:GLU:HG2   | 1.89                     | 0.55              |
| 3:D:909:ASN:O    | 3:D:910:SER:C     | 2.45                     | 0.55              |
| 3:D:930:LEU:O    | 3:D:933:ALA:HB3   | 2.07                     | 0.55              |
| 4:E:85:LEU:O     | 4:E:86:GLN:C      | 2.45                     | 0.55              |
| 5:F:368:VAL:CG2  | 5:F:369:LEU:H     | 2.14                     | 0.55              |
| 5:F:405:LEU:O    | 5:F:408:LEU:HB3   | 2.07                     | 0.55              |
| 2:M:237:ARG:O    | 2:M:240:THR:CB    | 2.55                     | 0.55              |
| 2:M:589:ARG:HG2  | 2:M:596:TYR:CZ    | 2.41                     | 0.55              |
| 2:M:719:PRO:HB3  | 2:M:820:ARG:NH1   | 2.21                     | 0.55              |
| 2:M:549:PHE:CD2  | 2:M:886:LEU:HB2   | 2.42                     | 0.55              |
| 3:N:27:GLU:HB2   | 3:N:28:LYS:CE     | 2.37                     | 0.55              |
| 3:N:280:ALA:HB1  | 3:N:282:TYR:CZ    | 2.42                     | 0.55              |
| 3:N:416:ALA:CB   | 3:N:432:TYR:CG    | 2.90                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:41:ARG:NH2   | 3:N:48:ARG:NH1    | 2.54                     | 0.55              |
| 3:N:356:PRO:CB   | 3:N:440:VAL:HB    | 2.34                     | 0.55              |
| 3:N:759:ALA:O    | 3:N:763:MET:HB2   | 2.06                     | 0.55              |
| 3:N:715:ALA:O    | 3:N:764:LEU:HD12  | 2.07                     | 0.55              |
| 2:M:780:GLU:HG2  | 5:P:379:ARG:HH21  | 1.69                     | 0.55              |
| 5:P:413:SER:CB   | 5:P:414:ARG:HH21  | 2.20                     | 0.55              |
| 1:B:112:ARG:NH2  | 1:B:125:PRO:C     | 2.60                     | 0.55              |
| 2:C:167:LYS:HB3  | 2:C:167:LYS:HZ3   | 1.72                     | 0.55              |
| 2:C:267:TYR:HE1  | 2:C:464:LEU:HD12  | 1.71                     | 0.55              |
| 2:C:439:CYS:HB2  | 2:C:541:SER:CB    | 2.35                     | 0.55              |
| 1:A:70:GLY:H     | 2:C:607:ASP:CB    | 2.20                     | 0.55              |
| 3:D:1095:THR:C   | 3:D:1099:VAL:HG23 | 2.27                     | 0.55              |
| 3:D:1179:GLU:C   | 3:D:1181:GLY:H    | 2.10                     | 0.55              |
| 3:D:1380:GLU:O   | 3:D:1418:LYS:N    | 2.30                     | 0.55              |
| 3:D:660:LYS:HD2  | 3:D:693:GLU:OE2   | 2.06                     | 0.55              |
| 4:E:6:ILE:CA     | 4:E:9:LEU:HD12    | 2.24                     | 0.55              |
| 5:F:260:ILE:HG13 | 5:F:261:PRO:HD2   | 1.88                     | 0.55              |
| 1:K:5:LYS:HZ2    | 1:K:29:GLU:N      | 2.05                     | 0.55              |
| 2:M:226:VAL:O    | 2:M:230:ARG:CZ    | 2.55                     | 0.55              |
| 2:M:23:VAL:HA    | 2:M:121:MET:CE    | 2.33                     | 0.55              |
| 2:M:486:MET:HG3  | 2:M:490:GLU:OE1   | 2.07                     | 0.55              |
| 3:N:1379:VAL:O   | 3:N:1393:GLN:N    | 2.40                     | 0.55              |
| 3:N:139:GLY:HA2  | 3:N:452:ILE:CG2   | 2.37                     | 0.55              |
| 3:N:186:VAL:HG12 | 3:N:187:LYS:N     | 2.22                     | 0.55              |
| 3:N:207:PHE:CZ   | 5:P:97:GLU:HB2    | 2.42                     | 0.55              |
| 3:N:238:PRO:HB3  | 3:N:317:VAL:C     | 2.28                     | 0.55              |
| 3:N:368:VAL:H    | 3:N:377:VAL:HB    | 1.71                     | 0.55              |
| 3:N:574:LEU:O    | 3:N:577:ALA:HB3   | 2.07                     | 0.55              |
| 3:N:628:ARG:N    | 3:N:648:MET:HE1   | 2.21                     | 0.55              |
| 3:N:795:VAL:HG13 | 3:N:879:ARG:HH12  | 1.71                     | 0.55              |
| 3:N:808:THR:N    | 3:N:809:PRO:CD    | 2.63                     | 0.55              |
| 3:N:812:ALA:HB2  | 3:N:816:HIS:HB2   | 1.89                     | 0.55              |
| 3:N:921:ARG:O    | 3:N:922:LEU:HD23  | 2.07                     | 0.55              |
| 3:N:988:ARG:HG2  | 3:N:992:ILE:HD11  | 1.87                     | 0.55              |
| 5:P:167:PRO:HB2  | 5:P:169:GLU:OE1   | 2.07                     | 0.55              |
| 5:P:192:LEU:O    | 5:P:196:VAL:HG23  | 2.06                     | 0.55              |
| 5:P:350:LEU:O    | 5:P:352:GLU:N     | 2.39                     | 0.55              |
| 5:P:400:ILE:O    | 5:P:401:GLU:C     | 2.45                     | 0.55              |
| 1:B:66:SER:O     | 1:B:75:VAL:HG23   | 2.07                     | 0.54              |
| 2:C:266:ARG:HB2  | 2:C:272:ALA:CB    | 2.36                     | 0.54              |
| 2:C:399:ASN:HB2  | 2:C:400:PRO:HD3   | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:41:ASN:HB2    | 2:C:45:GLN:C      | 2.28                     | 0.54              |
| 2:C:512:ARG:HG3   | 2:C:523:ILE:HD11  | 1.88                     | 0.54              |
| 3:D:1108:ARG:NE   | 3:D:1199:GLY:HA3  | 2.21                     | 0.54              |
| 3:D:1087:ARG:HD2  | 3:D:1234:THR:HA   | 1.89                     | 0.54              |
| 3:D:1083:ASP:HB2  | 3:D:1239:ARG:HH12 | 1.71                     | 0.54              |
| 3:D:489:ARG:HH21  | 3:D:1389:LEU:CD1  | 2.20                     | 0.54              |
| 3:D:1499:ARG:NH1  | 3:D:1499:ARG:HG3  | 2.22                     | 0.54              |
| 3:D:622:ARG:HG2   | 3:D:622:ARG:NH1   | 2.22                     | 0.54              |
| 3:D:984:THR:HG22  | 3:D:987:GLU:HB2   | 1.88                     | 0.54              |
| 5:F:224:VAL:O     | 5:F:225:GLU:C     | 2.46                     | 0.54              |
| 1:L:19:GLU:O      | 1:L:200:TRP:HA    | 2.07                     | 0.54              |
| 1:L:215:VAL:CG2   | 1:L:216:GLU:N     | 2.70                     | 0.54              |
| 1:K:34:VAL:HG11   | 1:L:42:ARG:HH12   | 1.71                     | 0.54              |
| 2:M:807:ARG:HB3   | 2:M:807:ARG:HH11  | 1.72                     | 0.54              |
| 3:N:1197:ARG:HG2  | 3:N:1198:TYR:CD2  | 2.41                     | 0.54              |
| 3:N:1267:ARG:CZ   | 3:N:1267:ARG:HB2  | 2.36                     | 0.54              |
| 3:N:259:VAL:O     | 3:N:260:GLU:HG3   | 2.07                     | 0.54              |
| 3:N:39:PRO:HG2    | 3:N:53:ILE:HD11   | 1.89                     | 0.54              |
| 3:N:582:LEU:O     | 3:N:603:LEU:HB2   | 2.07                     | 0.54              |
| 3:N:812:ALA:C     | 3:N:814:ALA:N     | 2.56                     | 0.54              |
| 3:N:966:GLU:HA    | 3:N:969:ARG:CZ    | 2.37                     | 0.54              |
| 5:P:367:MET:SD    | 5:P:371:LEU:HD11  | 2.46                     | 0.54              |
| 1:A:20:TYR:CD1    | 1:A:21:GLY:N      | 2.75                     | 0.54              |
| 2:C:1089:VAL:O    | 2:C:1093:GLN:HG3  | 2.08                     | 0.54              |
| 2:C:517:ARG:CB    | 2:C:520:GLU:HB2   | 2.35                     | 0.54              |
| 2:C:572:ILE:HG13  | 2:C:573:ARG:N     | 2.21                     | 0.54              |
| 3:D:539:ASP:O     | 3:D:542:ASP:HB2   | 2.07                     | 0.54              |
| 2:C:1031:ARG:N    | 3:D:622:ARG:HH12  | 2.05                     | 0.54              |
| 3:D:800:LYS:N     | 3:D:800:LYS:HE2   | 2.22                     | 0.54              |
| 3:D:851:LEU:H     | 3:D:851:LEU:HD23  | 1.70                     | 0.54              |
| 1:L:153:ALA:HB2   | 1:L:167:VAL:C     | 2.27                     | 0.54              |
| 1:L:28:LEU:CD2    | 1:L:29:GLU:H      | 2.20                     | 0.54              |
| 2:M:1058:ASP:HB3  | 2:M:1082:PRO:HB3  | 1.89                     | 0.54              |
| 2:M:224:GLU:HB3   | 2:M:227:PHE:CD1   | 2.42                     | 0.54              |
| 3:N:1137:ARG:O    | 3:N:1141:GLU:HG3  | 2.07                     | 0.54              |
| 3:N:1310:ARG:HB3  | 3:N:1327:ARG:HB2  | 1.88                     | 0.54              |
| 3:N:1101:VAL:HG21 | 3:N:1424:VAL:HB   | 1.87                     | 0.54              |
| 3:N:432:TYR:CD2   | 3:N:450:TYR:HB2   | 2.42                     | 0.54              |
| 3:N:500:ARG:O     | 3:N:504:ASP:N     | 2.33                     | 0.54              |
| 3:N:527:MET:HA    | 3:N:537:THR:CG2   | 2.37                     | 0.54              |
| 3:N:659:LYS:HG3   | 3:N:663:GLU:OE2   | 2.08                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:736:PHE:O     | 3:N:738:ALA:N    | 2.39                     | 0.54              |
| 3:N:807:ALA:HA    | 3:N:833:GLU:CB   | 2.36                     | 0.54              |
| 5:P:155:THR:HA    | 5:P:158:GLU:OE2  | 2.07                     | 0.54              |
| 5:P:265:VAL:O     | 5:P:266:GLU:C    | 2.46                     | 0.54              |
| 5:P:306:GLU:O     | 5:P:307:THR:C    | 2.45                     | 0.54              |
| 5:P:386:VAL:CG2   | 5:P:387:GLY:N    | 2.71                     | 0.54              |
| 1:B:224:TYR:HD2   | 1:B:224:TYR:N    | 2.06                     | 0.54              |
| 2:C:174:LEU:CD2   | 2:C:184:MET:HG2  | 2.37                     | 0.54              |
| 2:C:263:ASP:N     | 2:C:263:ASP:OD2  | 2.40                     | 0.54              |
| 2:C:640:ARG:HB2   | 2:C:642:ARG:NH2  | 2.23                     | 0.54              |
| 2:C:695:LEU:HD22  | 2:C:832:LYS:HE2  | 1.89                     | 0.54              |
| 2:C:808:ARG:H     | 2:C:815:LEU:HD11 | 1.72                     | 0.54              |
| 3:D:710:ARG:N     | 3:D:1227:GLN:OE1 | 2.31                     | 0.54              |
| 3:D:1087:ARG:HD2  | 3:D:1234:THR:C   | 2.27                     | 0.54              |
| 3:D:1483:PHE:N    | 3:D:1483:PHE:CD1 | 2.75                     | 0.54              |
| 3:D:1489:GLN:HA   | 3:D:1492:LEU:CD1 | 2.37                     | 0.54              |
| 3:D:185:VAL:HG23  | 3:D:203:ALA:H    | 1.73                     | 0.54              |
| 3:D:209:ARG:HA    | 3:D:347:VAL:HB   | 1.88                     | 0.54              |
| 3:D:253:ALA:N     | 3:D:301:GLY:CA   | 2.62                     | 0.54              |
| 3:D:238:PRO:HB3   | 3:D:318:ARG:HA   | 1.87                     | 0.54              |
| 3:D:827:ILE:CG2   | 3:D:837:GLY:HA3  | 2.36                     | 0.54              |
| 3:D:1486:VAL:HG22 | 4:E:75:PHE:HA    | 1.89                     | 0.54              |
| 1:K:103:ALA:O     | 1:K:104:GLU:HG3  | 2.07                     | 0.54              |
| 1:L:188:GLN:HG3   | 1:L:189:ARG:H    | 1.72                     | 0.54              |
| 2:M:1048:THR:O    | 2:M:1052:MET:HB2 | 2.06                     | 0.54              |
| 2:M:1061:GLU:HA   | 2:M:1064:ASN:ND2 | 2.22                     | 0.54              |
| 2:M:281:LEU:HB3   | 2:M:305:PRO:CB   | 2.37                     | 0.54              |
| 2:M:650:ARG:H     | 2:M:650:ARG:HE   | 0.72                     | 0.54              |
| 3:N:1281:VAL:HG23 | 3:N:1317:ASP:O   | 2.06                     | 0.54              |
| 3:N:288:MET:HE1   | 3:N:307:ALA:CB   | 2.35                     | 0.54              |
| 3:N:241:ILE:HG13  | 3:N:312:ARG:CZ   | 2.37                     | 0.54              |
| 3:N:90:MET:HE2    | 3:N:519:VAL:C    | 2.27                     | 0.54              |
| 5:P:253:ASP:CA    | 5:P:259:ARG:NH1  | 2.67                     | 0.54              |
| 1:A:123:MET:CE    | 1:A:123:MET:HA   | 2.37                     | 0.54              |
| 1:A:75:VAL:O      | 1:A:78:ILE:HB    | 2.07                     | 0.54              |
| 1:A:79:ILE:O      | 1:A:80:LEU:C     | 2.45                     | 0.54              |
| 1:B:112:ARG:CZ    | 1:B:112:ARG:HB3  | 2.38                     | 0.54              |
| 1:B:224:TYR:CD2   | 1:B:224:TYR:N    | 2.74                     | 0.54              |
| 1:B:76:VAL:CA     | 1:B:79:ILE:HD12  | 2.29                     | 0.54              |
| 2:C:1071:ILE:C    | 2:C:1073:GLY:H   | 2.11                     | 0.54              |
| 2:C:277:ALA:HB1   | 2:C:281:LEU:HD12 | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:305:PRO:O     | 2:C:308:ARG:HG2   | 2.07                     | 0.54              |
| 2:C:148:PHE:CZ    | 2:C:309:TYR:HD2   | 2.25                     | 0.54              |
| 2:C:512:ARG:CG    | 2:C:523:ILE:HD11  | 2.37                     | 0.54              |
| 2:C:556:ASN:O     | 2:C:559:LEU:HB3   | 2.07                     | 0.54              |
| 2:C:577:PRO:HA    | 2:C:671:ASN:OD1   | 2.08                     | 0.54              |
| 2:C:768:THR:HG22  | 2:C:770:GLU:N     | 2.23                     | 0.54              |
| 2:C:976:ASP:OD1   | 2:C:978:ARG:HG3   | 2.07                     | 0.54              |
| 3:D:1107:VAL:HG11 | 3:D:1217:ILE:HA   | 1.89                     | 0.54              |
| 3:D:1374:GLN:O    | 3:D:1377:LYS:HB3  | 2.05                     | 0.54              |
| 3:D:128:TYR:HE2   | 3:D:575:GLN:NE2   | 2.04                     | 0.54              |
| 2:C:1030:GLN:CG   | 3:D:626:SER:HB2   | 2.36                     | 0.54              |
| 3:D:803:GLY:C     | 3:D:805:GLU:N     | 2.61                     | 0.54              |
| 5:F:290:GLU:HA    | 5:F:293:GLU:OE1   | 2.07                     | 0.54              |
| 2:M:1100:GLN:CG   | 2:M:1102:LEU:HD21 | 2.36                     | 0.54              |
| 2:M:166:PRO:HB2   | 2:M:169:GLY:CA    | 2.37                     | 0.54              |
| 2:M:332:ARG:HG2   | 2:M:333:ILE:N     | 2.23                     | 0.54              |
| 2:M:630:ARG:HH11  | 2:M:630:ARG:HG2   | 1.72                     | 0.54              |
| 2:M:799:ILE:HD12  | 2:M:800:VAL:O     | 2.07                     | 0.54              |
| 3:N:1029:ARG:NH1  | 3:N:1029:ARG:HG3  | 2.22                     | 0.54              |
| 3:N:1032:PRO:O    | 3:N:1033:GLN:C    | 2.46                     | 0.54              |
| 3:N:996:TRP:CE3   | 3:N:1056:PRO:HG2  | 2.42                     | 0.54              |
| 5:P:370:LYS:HA    | 5:P:374:GLY:H     | 1.73                     | 0.54              |
| 5:P:98:GLU:O      | 5:P:99:GLU:C      | 2.46                     | 0.54              |
| 1:B:73:GLU:HB2    | 1:B:78:ILE:HD11   | 1.90                     | 0.54              |
| 2:C:1015:LEU:HD12 | 5:F:335:ASP:HB2   | 1.90                     | 0.54              |
| 2:C:212:GLY:HA3   | 2:C:218:VAL:HG11  | 1.89                     | 0.54              |
| 3:D:114:THR:HG22  | 3:D:114:THR:O     | 2.07                     | 0.54              |
| 3:D:1366:LYS:O    | 3:D:1369:GLU:N    | 2.41                     | 0.54              |
| 3:D:1462:LEU:HD22 | 3:D:1472:ILE:HD12 | 1.88                     | 0.54              |
| 3:D:268:ALA:HB3   | 3:D:290:PRO:HG3   | 1.90                     | 0.54              |
| 3:D:210:ARG:CB    | 3:D:389:GLU:HG3   | 2.35                     | 0.54              |
| 3:D:582:LEU:CA    | 3:D:603:LEU:HD12  | 2.16                     | 0.54              |
| 3:D:653:PHE:N     | 3:D:653:PHE:HD1   | 2.04                     | 0.54              |
| 3:D:706:PRO:HB2   | 3:D:708:LEU:CD2   | 2.36                     | 0.54              |
| 3:D:860:LEU:HA    | 3:D:877:PRO:CB    | 2.36                     | 0.54              |
| 3:D:925:GLU:CD    | 4:E:6:ILE:HG22    | 2.28                     | 0.54              |
| 3:D:984:THR:HG22  | 3:D:987:GLU:CB    | 2.38                     | 0.54              |
| 5:F:289:GLU:O     | 5:F:293:GLU:HG3   | 2.08                     | 0.54              |
| 1:L:161:ARG:CB    | 1:L:164:ALA:HB2   | 2.28                     | 0.54              |
| 1:L:176:ARG:HD2   | 1:L:200:TRP:NE1   | 2.21                     | 0.54              |
| 2:M:520:GLU:OE1   | 2:M:520:GLU:HA    | 2.06                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:554:ASP:HB2   | 2:M:880:MET:HB2   | 1.90                     | 0.54              |
| 3:N:1001:GLU:CA   | 3:N:1001:GLU:OE2  | 2.53                     | 0.54              |
| 3:N:1046:GLN:CA   | 3:N:1052:THR:HA   | 2.38                     | 0.54              |
| 3:N:1500:LYS:O    | 3:N:1503:VAL:HG23 | 2.08                     | 0.54              |
| 3:N:217:LYS:CD    | 3:N:262:LYS:HZ1   | 2.21                     | 0.54              |
| 3:N:441:ARG:C     | 3:N:443:VAL:N     | 2.59                     | 0.54              |
| 3:N:614:PHE:HZ    | 10:N:1528:NE6:H21 | 1.72                     | 0.54              |
| 4:O:71:GLY:O      | 4:O:73:LEU:N      | 2.41                     | 0.54              |
| 5:P:107:GLU:O     | 5:P:110:MET:HB3   | 2.07                     | 0.54              |
| 5:P:142:ARG:HD3   | 5:P:145:PRO:HA    | 1.90                     | 0.54              |
| 5:P:242:TRP:CA    | 5:P:245:GLN:HG2   | 2.35                     | 0.54              |
| 1:B:104:GLU:HB3   | 1:B:137:ARG:CB    | 2.37                     | 0.54              |
| 2:C:327:HIS:HA    | 2:C:431:HIS:NE2   | 2.22                     | 0.54              |
| 3:D:118:LEU:HD23  | 3:D:123:LEU:HD13  | 1.89                     | 0.54              |
| 3:D:1283:ILE:HD12 | 3:D:1315:ASP:OD2  | 2.07                     | 0.54              |
| 3:D:1315:ASP:O    | 3:D:1317:ASP:N    | 2.40                     | 0.54              |
| 3:D:560:GLN:HA    | 5:F:132:ARG:HH12  | 1.73                     | 0.54              |
| 2:C:1032:PHE:N    | 3:D:621:LYS:O     | 2.33                     | 0.54              |
| 3:D:730:PRO:HA    | 3:D:733:CYS:SG    | 2.48                     | 0.54              |
| 3:D:985:ASP:O     | 3:D:988:ARG:HB3   | 2.08                     | 0.54              |
| 4:E:27:ALA:O      | 4:E:31:LEU:HG     | 2.07                     | 0.54              |
| 2:M:136:ILE:HG21  | 2:M:336:VAL:HG13  | 1.90                     | 0.54              |
| 2:M:486:MET:SD    | 2:M:491:GLU:CA    | 2.96                     | 0.54              |
| 2:M:605:LYS:CB    | 2:M:610:ARG:NH2   | 2.70                     | 0.54              |
| 2:M:809:GLY:C     | 2:M:811:PRO:CD    | 2.74                     | 0.54              |
| 2:M:913:GLU:O     | 2:M:917:LEU:HG    | 2.08                     | 0.54              |
| 2:M:953:VAL:HG13  | 2:M:966:LEU:CD1   | 2.38                     | 0.54              |
| 3:N:1124:GLN:HG3  | 3:N:1133:ARG:HB3  | 1.88                     | 0.54              |
| 3:N:1120:VAL:N    | 3:N:1186:VAL:O    | 2.37                     | 0.54              |
| 3:N:154:THR:HG22  | 3:N:157:GLU:CD    | 2.27                     | 0.54              |
| 3:N:500:ARG:O     | 3:N:504:ASP:CB    | 2.56                     | 0.54              |
| 3:N:796:ARG:C     | 3:N:797:LYS:HG3   | 2.27                     | 0.54              |
| 3:N:959:GLU:O     | 3:N:962:GLN:HB2   | 2.07                     | 0.54              |
| 4:O:70:THR:O      | 4:O:72:ARG:N      | 2.40                     | 0.54              |
| 5:P:102:LEU:O     | 5:P:106:VAL:HG23  | 2.08                     | 0.54              |
| 5:P:365:GLU:HA    | 5:P:368:VAL:CG1   | 2.38                     | 0.54              |
| 1:B:58:ILE:HD13   | 1:B:59:GLU:N      | 2.23                     | 0.54              |
| 2:C:1013:TYR:O    | 2:C:1014:SER:C    | 2.46                     | 0.54              |
| 2:C:346:VAL:HB    | 2:C:350:ARG:NH2   | 2.23                     | 0.54              |
| 2:C:133:ASP:HB2   | 2:C:632:ASN:OD1   | 2.06                     | 0.54              |
| 2:C:694:LEU:CD2   | 2:C:868:ASP:HB3   | 2.30                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:915:LYS:HD3   | 2:C:968:LEU:O     | 2.07                     | 0.54              |
| 2:C:73:LEU:CB     | 2:C:93:PRO:O      | 2.56                     | 0.54              |
| 2:C:953:VAL:HG12  | 2:C:965:GLU:HB3   | 1.88                     | 0.54              |
| 2:C:889:HIS:HD2   | 2:C:970:GLY:HA3   | 1.71                     | 0.54              |
| 3:D:109:PRO:HG2   | 3:D:111:LYS:CE    | 2.38                     | 0.54              |
| 3:D:1354:LYS:HA   | 3:D:1357:ARG:HD2  | 1.90                     | 0.54              |
| 3:D:154:THR:HG23  | 3:D:156:GLU:OE2   | 2.08                     | 0.54              |
| 3:D:177:ALA:HB3   | 3:D:191:LEU:O     | 2.07                     | 0.54              |
| 3:D:349:PRO:CG    | 5:F:97:GLU:HG2    | 2.37                     | 0.54              |
| 1:K:57:TYR:HE1    | 1:K:163:ASN:HB2   | 1.73                     | 0.54              |
| 2:M:1086:ARG:HD3  | 2:M:1112:PHE:CD2  | 2.42                     | 0.54              |
| 2:M:151:ASP:HB2   | 2:M:158:TYR:HA    | 1.89                     | 0.54              |
| 2:M:389:SER:HB3   | 2:M:392:SER:CB    | 2.38                     | 0.54              |
| 2:M:396:ASP:HB2   | 2:M:406:HIS:CD2   | 2.43                     | 0.54              |
| 2:M:672:VAL:HG23  | 2:M:868:ASP:OD2   | 2.08                     | 0.54              |
| 2:M:896:PHE:O     | 2:M:898:GLY:N     | 2.40                     | 0.54              |
| 3:N:147:VAL:CG2   | 3:N:148:GLU:N     | 2.56                     | 0.54              |
| 3:N:154:THR:HG23  | 3:N:156:GLU:OE2   | 2.08                     | 0.54              |
| 3:N:59:ALA:HB3    | 3:N:76:CYS:HB2    | 1.89                     | 0.54              |
| 3:N:792:ILE:HD13  | 3:N:941:PHE:CE1   | 2.42                     | 0.54              |
| 1:A:83:LYS:NZ     | 1:A:170:VAL:HG22  | 2.23                     | 0.54              |
| 2:C:30:LEU:HD23   | 2:C:44:ILE:CD1    | 2.38                     | 0.54              |
| 2:C:133:ASP:HB3   | 2:C:395:LYS:HB3   | 1.90                     | 0.54              |
| 2:C:498:GLN:OE1   | 3:D:1067:VAL:HG13 | 2.07                     | 0.54              |
| 2:C:895:TYR:CD2   | 2:C:895:TYR:C     | 2.81                     | 0.54              |
| 3:D:1311:LEU:CG   | 3:D:1312:LEU:N    | 2.71                     | 0.54              |
| 3:D:167:GLU:HB3   | 3:D:169:TYR:CE1   | 2.43                     | 0.54              |
| 3:D:604:THR:O     | 3:D:607:LEU:HB3   | 2.07                     | 0.54              |
| 3:D:794:GLN:OE1   | 3:D:905:PRO:HG3   | 2.06                     | 0.54              |
| 2:M:1088:LEU:CA   | 2:M:1091:GLU:OE1  | 2.52                     | 0.54              |
| 2:M:252:LYS:HD3   | 2:M:298:PHE:CE1   | 2.43                     | 0.54              |
| 2:M:603:VAL:CG1   | 2:M:645:VAL:HA    | 2.37                     | 0.54              |
| 2:M:808:ARG:NH2   | 2:M:819:VAL:O     | 2.40                     | 0.54              |
| 2:M:983:ILE:O     | 2:M:984:GLU:C     | 2.46                     | 0.54              |
| 3:N:1476:THR:HG21 | 4:O:20:THR:HB     | 1.89                     | 0.54              |
| 3:N:1486:VAL:HG13 | 4:O:74:VAL:O      | 2.08                     | 0.54              |
| 3:N:564:GLU:CD    | 3:N:565:ILE:N     | 2.61                     | 0.54              |
| 3:N:84:ILE:HG23   | 3:N:85:VAL:N      | 2.22                     | 0.54              |
| 3:N:1216:SER:CB   | 4:O:16:LYS:H      | 2.20                     | 0.54              |
| 3:N:570:GLU:OE2   | 5:P:214:GLN:HG3   | 2.07                     | 0.54              |
| 1:A:11:PHE:HB2    | 1:A:25:LEU:HD13   | 1.90                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1:MET:N      | 1:A:6:LEU:HB2     | 2.21                     | 0.54              |
| 1:B:117:VAL:CG1  | 1:B:118:ALA:N     | 2.70                     | 0.54              |
| 1:B:56:VAL:HG12  | 1:B:57:TYR:N      | 2.21                     | 0.54              |
| 2:C:159:ILE:HG22 | 2:C:174:LEU:O     | 2.08                     | 0.54              |
| 2:C:24:GLU:HA    | 2:C:27:ARG:HB3    | 1.88                     | 0.54              |
| 2:C:533:ASP:HB3  | 2:C:538:GLN:OE1   | 2.08                     | 0.54              |
| 2:C:595:LEU:HD21 | 2:C:639:GLN:NE2   | 2.23                     | 0.54              |
| 1:A:72:LYS:O     | 2:C:608:GLY:HA2   | 2.08                     | 0.54              |
| 2:C:685:GLU:CG   | 3:D:739:ASP:HB3   | 2.37                     | 0.54              |
| 3:D:1121:PRO:O   | 3:D:1122:LEU:HD23 | 2.07                     | 0.54              |
| 3:D:1404:ASN:HA  | 3:D:1409:ALA:H    | 1.70                     | 0.54              |
| 3:D:153:LEU:CD1  | 3:D:157:GLU:HB3   | 2.38                     | 0.54              |
| 3:D:287:GLY:C    | 3:D:311:LEU:HD22  | 2.28                     | 0.54              |
| 3:D:564:GLU:HA   | 3:D:567:ILE:HB    | 1.88                     | 0.54              |
| 3:D:592:THR:CG2  | 3:D:600:LEU:HD21  | 2.38                     | 0.54              |
| 3:D:65:ARG:HG2   | 3:D:67:ARG:HG2    | 1.89                     | 0.54              |
| 3:D:6:ARG:HH21   | 3:D:1482:ARG:HH22 | 1.56                     | 0.54              |
| 3:D:819:GLY:HA2  | 3:D:824:ASN:ND2   | 2.23                     | 0.54              |
| 3:D:955:VAL:O    | 3:D:957:PRO:HD3   | 2.08                     | 0.54              |
| 3:D:996:TRP:O    | 3:D:997:THR:C     | 2.46                     | 0.54              |
| 4:E:88:GLU:OE1   | 4:E:91:ARG:NH1    | 2.41                     | 0.54              |
| 1:L:112:ARG:HH12 | 1:L:125:PRO:HB2   | 1.72                     | 0.54              |
| 2:M:449:ILE:HD13 | 3:N:1082:ALA:HA   | 1.90                     | 0.54              |
| 2:M:861:LEU:HB2  | 2:M:863:ASP:OD1   | 2.08                     | 0.54              |
| 3:N:1112:CYS:N   | 3:N:1201:CYS:CB   | 2.70                     | 0.54              |
| 3:N:1123:PHE:HA  | 3:N:1133:ARG:O    | 2.08                     | 0.54              |
| 3:N:1216:SER:HB2 | 4:O:16:LYS:H      | 1.71                     | 0.54              |
| 3:N:1395:LEU:O   | 3:N:1398:TRP:CD1  | 2.61                     | 0.54              |
| 3:N:692:GLU:O    | 3:N:693:GLU:C     | 2.45                     | 0.54              |
| 3:N:806:PHE:CD2  | 3:N:809:PRO:HB2   | 2.43                     | 0.54              |
| 3:N:924:MET:CG   | 3:N:925:GLU:N     | 2.71                     | 0.54              |
| 3:N:411:THR:CG2  | 5:P:179:GLU:HG3   | 2.26                     | 0.54              |
| 5:P:329:TYR:O    | 5:P:332:PHE:CD1   | 2.61                     | 0.54              |
| 1:A:123:MET:HE2  | 1:A:123:MET:HA    | 1.89                     | 0.54              |
| 1:A:152:PRO:O    | 1:A:155:LYS:CB    | 2.56                     | 0.54              |
| 2:C:10:ARG:NH1   | 2:C:481:ASP:OD1   | 2.41                     | 0.54              |
| 2:C:289:THR:O    | 2:C:290:LEU:HD23  | 2.08                     | 0.54              |
| 2:C:943:VAL:O    | 2:C:946:ARG:N     | 2.41                     | 0.54              |
| 3:D:1123:PHE:HA  | 3:D:1133:ARG:O    | 2.08                     | 0.54              |
| 3:D:1311:LEU:HG  | 3:D:1313:VAL:H    | 1.73                     | 0.54              |
| 3:D:1360:GLY:HA2 | 3:D:1362:LYS:NZ   | 2.23                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:437:VAL:HG13  | 3:D:437:VAL:O     | 2.06                     | 0.54              |
| 3:D:441:ARG:HB3   | 3:D:443:VAL:HG23  | 1.89                     | 0.54              |
| 3:D:414:ARG:HH11  | 3:D:451:ASP:CG    | 2.11                     | 0.54              |
| 3:D:136:ASP:OD2   | 3:D:455:ARG:HD2   | 2.08                     | 0.54              |
| 3:D:489:ARG:HH21  | 3:D:1389:LEU:HD12 | 1.73                     | 0.54              |
| 3:D:541:ASN:O     | 3:D:545:ARG:HG3   | 2.08                     | 0.54              |
| 3:D:630:VAL:HA    | 3:D:744:GLN:HA    | 1.89                     | 0.54              |
| 3:D:887:ALA:HA    | 3:D:890:VAL:HG22  | 1.90                     | 0.54              |
| 1:L:20:TYR:HA     | 1:L:199:ILE:O     | 2.06                     | 0.54              |
| 2:M:185:LYS:NZ    | 2:M:190:LYS:NZ    | 2.56                     | 0.54              |
| 2:M:492:ASP:HA    | 2:M:518:LYS:HB3   | 1.90                     | 0.54              |
| 3:N:127:LEU:HD23  | 3:N:128:TYR:HA    | 1.89                     | 0.54              |
| 3:N:1102:THR:HG22 | 3:N:1374:GLN:HG3  | 1.89                     | 0.54              |
| 3:N:1478:SER:C    | 3:N:1482:ARG:HG3  | 2.29                     | 0.54              |
| 3:N:14:SER:HB3    | 3:N:16:GLU:OE2    | 2.08                     | 0.54              |
| 3:N:499:VAL:HG12  | 3:N:503:LEU:HD12  | 1.90                     | 0.54              |
| 3:N:87:ARG:HG3    | 3:N:88:TYR:CE2    | 2.43                     | 0.54              |
| 5:P:221:ILE:O     | 5:P:224:VAL:HB    | 2.08                     | 0.54              |
| 5:P:95:THR:O      | 5:P:96:LEU:C      | 2.46                     | 0.54              |
| 1:A:127:LEU:HD12  | 1:A:128:HIS:N     | 2.23                     | 0.53              |
| 1:A:200:TRP:N     | 1:A:200:TRP:CD1   | 2.76                     | 0.53              |
| 1:B:181:VAL:HG22  | 1:B:195:LEU:HD13  | 1.90                     | 0.53              |
| 2:C:343:GLN:HG2   | 2:C:385:PHE:CG    | 2.44                     | 0.53              |
| 2:C:599:GLU:HG3   | 2:C:600:ASP:H     | 1.72                     | 0.53              |
| 2:C:649:VAL:CG1   | 2:C:653:ASP:HB2   | 2.38                     | 0.53              |
| 2:C:685:GLU:HG2   | 3:D:739:ASP:HB3   | 1.90                     | 0.53              |
| 2:C:674:VAL:HB    | 2:C:869:VAL:HG13  | 1.89                     | 0.53              |
| 2:C:994:ILE:CG2   | 2:C:995:MET:N     | 2.70                     | 0.53              |
| 3:D:1092:GLY:O    | 3:D:1093:TYR:C    | 2.46                     | 0.53              |
| 3:D:109:PRO:O     | 3:D:111:LYS:HE3   | 2.08                     | 0.53              |
| 3:D:1481:VAL:HG12 | 4:E:21:VAL:HG21   | 1.88                     | 0.53              |
| 3:D:169:TYR:O     | 3:D:392:SER:HA    | 2.08                     | 0.53              |
| 3:D:625:TYR:O     | 3:D:749:VAL:HG23  | 2.08                     | 0.53              |
| 3:D:768:ASN:C     | 3:D:769:LEU:HD12  | 2.28                     | 0.53              |
| 2:C:984:GLU:HG3   | 3:D:944:THR:O     | 2.08                     | 0.53              |
| 5:F:365:GLU:HA    | 5:F:368:VAL:CG1   | 2.36                     | 0.53              |
| 1:K:20:TYR:C      | 1:K:207:PRO:HG2   | 2.28                     | 0.53              |
| 1:L:150:TYR:CZ    | 1:L:168:ASP:HB3   | 2.42                     | 0.53              |
| 2:M:166:PRO:HG2   | 2:M:262:ALA:O     | 2.08                     | 0.53              |
| 2:M:299:LYS:HG2   | 2:M:300:ASP:N     | 2.23                     | 0.53              |
| 2:M:517:ARG:O     | 2:M:520:GLU:HG2   | 2.07                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:649:VAL:CG1   | 2:M:653:ASP:HB2   | 2.38                     | 0.53              |
| 3:N:1205:TYR:HD2  | 3:N:1215:VAL:HG11 | 1.73                     | 0.53              |
| 3:N:133:ILE:HD12  | 3:N:456:MET:HE1   | 1.89                     | 0.53              |
| 3:N:654:LYS:CB    | 3:N:655:PRO:HD3   | 2.30                     | 0.53              |
| 4:O:85:LEU:H      | 4:O:85:LEU:HD23   | 1.72                     | 0.53              |
| 5:P:223:ALA:HB2   | 5:P:242:TRP:CB    | 2.38                     | 0.53              |
| 5:P:256:ARG:HB3   | 5:P:258:ILE:O     | 2.07                     | 0.53              |
| 5:P:301:ALA:O     | 5:P:304:VAL:HB    | 2.08                     | 0.53              |
| 5:P:308:LEU:H     | 5:P:308:LEU:CD2   | 2.21                     | 0.53              |
| 1:A:189:ARG:HA    | 11:A:317:HOH:O    | 2.08                     | 0.53              |
| 1:A:228:PRO:C     | 1:A:229:GLN:HG3   | 2.28                     | 0.53              |
| 1:A:75:VAL:O      | 1:A:79:ILE:HG13   | 2.08                     | 0.53              |
| 1:B:206:THR:CG2   | 1:B:208:LEU:HB3   | 2.38                     | 0.53              |
| 1:B:56:VAL:HG22   | 1:B:142:VAL:HG13  | 1.90                     | 0.53              |
| 2:C:1104:GLU:C    | 2:C:1106:ASP:H    | 2.10                     | 0.53              |
| 2:C:254:VAL:HB    | 2:C:258:TYR:CE1   | 2.43                     | 0.53              |
| 2:C:384:GLU:HA    | 2:C:388:ARG:HH21  | 1.74                     | 0.53              |
| 2:C:461:VAL:HA    | 2:C:466:PHE:O     | 2.08                     | 0.53              |
| 2:C:603:VAL:CG2   | 2:C:647:GLN:HB3   | 2.37                     | 0.53              |
| 2:C:666:LEU:HD12  | 2:C:667:ALA:H     | 1.72                     | 0.53              |
| 2:C:728:HIS:CG    | 2:C:729:LEU:N     | 2.77                     | 0.53              |
| 2:C:5:ARG:HG2     | 2:C:902:ILE:HD12  | 1.90                     | 0.53              |
| 3:D:119:SER:C     | 3:D:121:THR:N     | 2.60                     | 0.53              |
| 3:D:1216:SER:OG   | 4:E:16:LYS:HB3    | 2.09                     | 0.53              |
| 3:D:1277:ILE:HG21 | 3:D:1299:PHE:CE1  | 2.43                     | 0.53              |
| 3:D:215:TYR:CE1   | 3:D:380:GLU:HB2   | 2.43                     | 0.53              |
| 3:D:351:MET:HA    | 3:D:370:ALA:HB2   | 1.89                     | 0.53              |
| 3:D:448:GLU:N     | 3:D:448:GLU:OE1   | 2.42                     | 0.53              |
| 3:D:958:GLU:OE2   | 3:D:961:LYS:HG3   | 2.08                     | 0.53              |
| 2:C:1102:LEU:CD1  | 3:D:9:ARG:HB2     | 2.39                     | 0.53              |
| 4:E:26:ARG:O      | 4:E:30:LEU:HB2    | 2.08                     | 0.53              |
| 4:E:46:PRO:HG2    | 4:E:63:TRP:CD1    | 2.44                     | 0.53              |
| 5:F:272:SER:O     | 5:F:275:ALA:HB3   | 2.08                     | 0.53              |
| 2:M:292:ARG:HE    | 2:M:295:ASP:HB3   | 1.71                     | 0.53              |
| 2:M:622:GLU:O     | 2:M:624:PRO:HD3   | 2.08                     | 0.53              |
| 2:M:738:ASP:OD2   | 2:M:739:GLU:OE2   | 2.26                     | 0.53              |
| 2:M:672:VAL:CG2   | 2:M:868:ASP:HB2   | 2.38                     | 0.53              |
| 2:M:998:TYR:HE2   | 2:M:1000:MET:HA   | 1.72                     | 0.53              |
| 3:N:1435:LEU:O    | 3:N:1438:ALA:N    | 2.41                     | 0.53              |
| 3:N:10:ILE:O      | 3:N:1451:ALA:HA   | 2.08                     | 0.53              |
| 3:N:163:TYR:OH    | 5:P:186:HIS:CE1   | 2.61                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:411:THR:H     | 3:N:437:VAL:CG2  | 2.21                     | 0.53              |
| 3:N:734:GLU:OE2   | 3:N:780:LYS:NZ   | 2.38                     | 0.53              |
| 3:N:799:LYS:HB2   | 3:N:826:PRO:HG2  | 1.89                     | 0.53              |
| 3:N:817:GLU:O     | 3:N:821:VAL:HG23 | 2.07                     | 0.53              |
| 3:N:841:TYR:HB2   | 3:N:864:VAL:CG1  | 2.34                     | 0.53              |
| 3:N:894:LYS:O     | 3:N:898:GLU:HG3  | 2.08                     | 0.53              |
| 3:N:915:VAL:O     | 3:N:918:ALA:HB3  | 2.07                     | 0.53              |
| 3:N:989:TYR:CZ    | 3:N:993:LEU:HD11 | 2.43                     | 0.53              |
| 1:A:30:ARG:HH21   | 1:A:191:ASP:CB   | 2.22                     | 0.53              |
| 1:A:70:GLY:N      | 2:C:607:ASP:HB2  | 2.22                     | 0.53              |
| 2:C:141:HIS:CD2   | 2:C:334:ARG:HG2  | 2.43                     | 0.53              |
| 2:C:397:GLU:HA    | 2:C:403:SER:HB3  | 1.89                     | 0.53              |
| 2:C:571:LEU:CD1   | 2:C:700:TYR:HA   | 2.39                     | 0.53              |
| 2:C:603:VAL:CG1   | 2:C:645:VAL:HA   | 2.38                     | 0.53              |
| 2:C:634:GLY:HA3   | 2:C:704:HIS:CE1  | 2.42                     | 0.53              |
| 3:D:1045:MET:O    | 3:D:1053:PHE:HD1 | 1.91                     | 0.53              |
| 3:D:1286:THR:HG22 | 3:D:1288:GLU:N   | 2.21                     | 0.53              |
| 3:D:1447:LEU:O    | 3:D:1448:THR:C   | 2.47                     | 0.53              |
| 3:D:325:GLU:HG2   | 3:D:332:TYR:HB3  | 1.91                     | 0.53              |
| 3:D:414:ARG:HA    | 3:D:433:GLY:O    | 2.09                     | 0.53              |
| 3:D:703:ASN:HD22  | 3:D:704:ARG:H    | 1.56                     | 0.53              |
| 3:D:937:TYR:CD1   | 3:D:937:TYR:N    | 2.77                     | 0.53              |
| 5:F:287:THR:O     | 5:F:288:TYR:C    | 2.46                     | 0.53              |
| 1:K:122:ILE:HG22  | 1:K:124:ASN:N    | 2.11                     | 0.53              |
| 1:K:5:LYS:C       | 1:K:7:LYS:H      | 2.11                     | 0.53              |
| 1:K:9:PRO:HB2     | 1:K:25:LEU:HD11  | 1.90                     | 0.53              |
| 1:L:144:VAL:HG12  | 1:L:145:ASP:H    | 1.73                     | 0.53              |
| 2:M:101:ILE:HA    | 2:M:106:GLY:O    | 2.08                     | 0.53              |
| 2:M:140:ILE:HD12  | 2:M:331:ARG:NH2  | 2.23                     | 0.53              |
| 2:M:355:VAL:HA    | 2:M:358:ARG:NE   | 2.23                     | 0.53              |
| 2:M:923:GLU:O     | 2:M:924:VAL:C    | 2.47                     | 0.53              |
| 2:M:926:PHE:HE2   | 2:M:960:GLU:HG3  | 1.74                     | 0.53              |
| 2:M:69:LEU:HB3    | 2:M:97:ARG:CB    | 2.39                     | 0.53              |
| 3:N:1032:PRO:O    | 3:N:1035:ILE:N   | 2.41                     | 0.53              |
| 3:N:1171:VAL:O    | 3:N:1172:HIS:C   | 2.46                     | 0.53              |
| 3:N:124:GLU:HG3   | 3:N:128:TYR:CZ   | 2.44                     | 0.53              |
| 3:N:1465:ASN:ND2  | 3:N:1472:ILE:HA  | 2.23                     | 0.53              |
| 3:N:238:PRO:CG    | 3:N:318:ARG:HG2  | 2.38                     | 0.53              |
| 3:N:626:SER:HA    | 3:N:747:VAL:O    | 2.09                     | 0.53              |
| 2:M:1005:MET:HE1  | 3:N:648:MET:HB2  | 1.89                     | 0.53              |
| 3:N:821:VAL:C     | 3:N:823:LEU:H    | 2.11                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:P:352:GLU:O    | 5:P:353:GLU:C    | 2.46                     | 0.53              |
| 5:P:81:VAL:CG2   | 5:P:82:ARG:H     | 2.19                     | 0.53              |
| 1:A:150:TYR:HD1  | 1:A:170:VAL:HG12 | 1.73                     | 0.53              |
| 1:A:36:LEU:C     | 1:A:40:LEU:HD12  | 2.28                     | 0.53              |
| 1:B:19:GLU:HG2   | 1:B:203:GLY:N    | 2.23                     | 0.53              |
| 2:C:208:ALA:HB2  | 2:C:221:LEU:HD22 | 1.90                     | 0.53              |
| 2:C:396:ASP:OD1  | 2:C:402:SER:HB2  | 2.09                     | 0.53              |
| 2:C:91:GLN:HB3   | 2:C:119:PRO:HA   | 1.90                     | 0.53              |
| 3:D:250:LEU:CD1  | 3:D:304:LEU:HA   | 2.39                     | 0.53              |
| 3:D:397:LYS:O    | 3:D:447:VAL:HG13 | 2.09                     | 0.53              |
| 3:D:434:ARG:HH21 | 3:D:451:ASP:CG   | 2.10                     | 0.53              |
| 3:D:436:GLU:HB2  | 3:D:445:ARG:O    | 2.09                     | 0.53              |
| 3:D:639:LEU:N    | 3:D:729:HIS:CE1  | 2.76                     | 0.53              |
| 3:D:812:ALA:CA   | 3:D:816:HIS:HB2  | 2.26                     | 0.53              |
| 3:D:972:LEU:HD23 | 3:D:972:LEU:H    | 1.71                     | 0.53              |
| 5:F:231:ARG:HB2  | 5:F:233:PHE:CZ   | 2.44                     | 0.53              |
| 5:F:353:GLU:HA   | 5:F:356:LYS:CD   | 2.38                     | 0.53              |
| 5:F:82:ARG:O     | 5:F:85:LEU:HB2   | 2.09                     | 0.53              |
| 1:K:69:PRO:O     | 1:K:71:VAL:HG23  | 2.06                     | 0.53              |
| 1:L:182:GLU:O    | 1:L:194:LYS:HB3  | 2.08                     | 0.53              |
| 2:M:41:ASN:HD22  | 2:M:42:VAL:N     | 2.05                     | 0.53              |
| 2:M:437:ARG:HG3  | 2:M:437:ARG:HH11 | 1.73                     | 0.53              |
| 2:M:572:ILE:HG13 | 2:M:701:THR:O    | 2.09                     | 0.53              |
| 2:M:603:VAL:CG2  | 2:M:647:GLN:HB3  | 2.38                     | 0.53              |
| 2:M:774:LEU:C    | 2:M:774:LEU:HD13 | 2.29                     | 0.53              |
| 3:N:363:ALA:HA   | 3:N:380:GLU:HA   | 1.90                     | 0.53              |
| 3:N:372:ASP:C    | 3:N:374:GLU:N    | 2.61                     | 0.53              |
| 5:P:110:MET:HG2  | 5:P:111:GLU:N    | 2.23                     | 0.53              |
| 5:P:132:ARG:HG2  | 5:P:181:GLU:HG2  | 1.90                     | 0.53              |
| 5:P:208:SER:HB3  | 5:P:211:ASP:CG   | 2.29                     | 0.53              |
| 5:P:95:THR:O     | 5:P:98:GLU:HB2   | 2.08                     | 0.53              |
| 1:B:9:PRO:HA     | 1:B:27:PRO:HD2   | 1.90                     | 0.53              |
| 2:C:1048:THR:O   | 2:C:1052:MET:HB2 | 2.08                     | 0.53              |
| 2:C:841:ASN:CG   | 2:C:845:ASN:HB3  | 2.29                     | 0.53              |
| 3:D:956:ILE:HG12 | 3:D:1039:CYS:O   | 2.08                     | 0.53              |
| 3:D:1400:VAL:O   | 3:D:1404:ASN:ND2 | 2.42                     | 0.53              |
| 3:D:218:LYS:HA   | 3:D:337:LEU:O    | 2.09                     | 0.53              |
| 3:D:56:TYR:H     | 3:D:81:THR:C     | 2.11                     | 0.53              |
| 3:D:591:VAL:HG11 | 3:D:597:ASP:O    | 2.09                     | 0.53              |
| 3:D:984:THR:CG2  | 3:D:987:GLU:H    | 2.21                     | 0.53              |
| 2:M:94:LEU:N     | 2:M:116:GLY:O    | 2.40                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:603:VAL:HG21  | 2:M:647:GLN:HB3  | 1.89                     | 0.53              |
| 2:M:625:LEU:CD1   | 2:M:639:GLN:HB2  | 2.37                     | 0.53              |
| 3:N:1031:ASN:OD1  | 3:N:1034:GLN:HG3 | 2.09                     | 0.53              |
| 3:N:124:GLU:O     | 3:N:125:GLN:C    | 2.47                     | 0.53              |
| 3:N:1287:GLU:HB3  | 3:N:1288:GLU:OE1 | 2.09                     | 0.53              |
| 3:N:1396:GLU:C    | 3:N:1398:TRP:N   | 2.61                     | 0.53              |
| 3:N:99:ALA:O      | 3:N:514:LEU:HB2  | 2.08                     | 0.53              |
| 3:N:99:ALA:N      | 3:N:514:LEU:O    | 2.39                     | 0.53              |
| 3:N:530:VAL:O     | 3:N:531:ASP:C    | 2.47                     | 0.53              |
| 5:P:403:LYS:NZ    | 5:P:407:LYS:HE2  | 2.22                     | 0.53              |
| 5:P:410:TYR:O     | 5:P:413:SER:HB2  | 2.09                     | 0.53              |
| 1:A:214:ALA:HA    | 1:A:217:ILE:HD12 | 1.91                     | 0.53              |
| 1:B:210:ALA:O     | 1:B:211:LEU:C    | 2.46                     | 0.53              |
| 1:B:75:VAL:O      | 1:B:79:ILE:HG13  | 2.08                     | 0.53              |
| 2:C:204:GLN:C     | 2:C:209:ARG:HD3  | 2.28                     | 0.53              |
| 2:C:293:PHE:CD1   | 2:C:294:GLU:N    | 2.77                     | 0.53              |
| 2:C:329:GLY:CA    | 2:C:488:ALA:HB3  | 2.38                     | 0.53              |
| 2:C:571:LEU:HD11  | 2:C:700:TYR:HA   | 1.90                     | 0.53              |
| 2:C:772:ARG:HD3   | 5:F:373:LYS:HD2  | 1.89                     | 0.53              |
| 2:C:806:LEU:HB2   | 2:C:822:VAL:CG2  | 2.38                     | 0.53              |
| 2:C:87:ASP:OD1    | 2:C:824:ARG:NH2  | 2.40                     | 0.53              |
| 3:D:1119:SER:HB3  | 3:D:1185:GLU:HB3 | 1.91                     | 0.53              |
| 3:D:1232:PRO:HB2  | 3:D:1356:TYR:HE2 | 1.74                     | 0.53              |
| 3:D:1286:THR:HB   | 3:D:1289:LYS:N   | 2.23                     | 0.53              |
| 3:D:1436:SER:O    | 3:D:1439:SER:HB3 | 2.08                     | 0.53              |
| 3:D:154:THR:H     | 3:D:157:GLU:CD   | 2.12                     | 0.53              |
| 3:D:244:GLU:OE2   | 3:D:310:LEU:HD23 | 2.08                     | 0.53              |
| 3:D:812:ALA:O     | 3:D:813:LEU:C    | 2.46                     | 0.53              |
| 2:C:983:ILE:HG23  | 3:D:944:THR:O    | 2.08                     | 0.53              |
| 3:D:9:ARG:CG      | 3:D:10:ILE:N     | 2.71                     | 0.53              |
| 5:F:94:LEU:CG     | 5:F:190:ALA:HB1  | 2.38                     | 0.53              |
| 1:L:83:LYS:HE2    | 1:L:168:ASP:HB2  | 1.91                     | 0.53              |
| 1:L:176:ARG:HG2   | 1:L:177:VAL:H    | 1.71                     | 0.53              |
| 1:L:186:LEU:C     | 1:L:188:GLN:H    | 2.11                     | 0.53              |
| 1:L:90:LEU:O      | 1:L:92:PRO:HD3   | 2.08                     | 0.53              |
| 2:M:1030:GLN:NE2  | 3:N:628:ARG:HH21 | 2.05                     | 0.53              |
| 2:M:573:ARG:HB2   | 2:M:670:GLN:NE2  | 2.23                     | 0.53              |
| 3:N:1094:LEU:HD23 | 3:N:1230:GLY:HA2 | 1.91                     | 0.53              |
| 3:N:125:GLN:O     | 3:N:126:VAL:C    | 2.47                     | 0.53              |
| 3:N:1371:VAL:O    | 3:N:1374:GLN:HB2 | 2.09                     | 0.53              |
| 3:N:1101:VAL:CG2  | 3:N:1428:ALA:HB2 | 2.21                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:139:GLY:HA3  | 3:N:147:VAL:CG2   | 2.38                     | 0.53              |
| 3:N:259:VAL:HG23 | 3:N:270:LEU:HD11  | 1.89                     | 0.53              |
| 3:N:538:SER:OG   | 3:N:540:LEU:HG    | 2.09                     | 0.53              |
| 2:M:1010:THR:HA  | 3:N:624:ASP:OD1   | 2.09                     | 0.53              |
| 5:P:110:MET:HG2  | 5:P:114:LYS:HE3   | 1.90                     | 0.53              |
| 5:P:239:ALA:O    | 5:P:240:THR:C     | 2.46                     | 0.53              |
| 1:B:138:LEU:HD11 | 1:B:140:MET:HE2   | 1.90                     | 0.53              |
| 1:B:153:ALA:HB2  | 1:B:167:VAL:C     | 2.29                     | 0.53              |
| 2:C:1048:THR:O   | 2:C:1052:MET:N    | 2.36                     | 0.53              |
| 2:C:135:VAL:CG2  | 2:C:395:LYS:HA    | 2.38                     | 0.53              |
| 2:C:193:LEU:HD12 | 2:C:196:LEU:CD1   | 2.36                     | 0.53              |
| 2:C:263:ASP:HB2  | 2:C:264:PRO:HD3   | 1.89                     | 0.53              |
| 2:C:34:VAL:N     | 2:C:35:PRO:HD3    | 2.23                     | 0.53              |
| 2:C:545:ASN:CB   | 2:C:583:LEU:HD11  | 2.38                     | 0.53              |
| 2:C:591:SER:O    | 2:C:592:LEU:HB2   | 2.09                     | 0.53              |
| 2:C:695:LEU:O    | 2:C:832:LYS:NZ    | 2.33                     | 0.53              |
| 2:C:897:LEU:HD13 | 2:C:917:LEU:HD22  | 1.90                     | 0.53              |
| 3:D:1302:GLU:HG2 | 3:D:1303:TYR:N    | 2.23                     | 0.53              |
| 3:D:432:TYR:N    | 3:D:432:TYR:CD1   | 2.76                     | 0.53              |
| 3:D:546:ARG:HH21 | 3:D:577:ALA:CA    | 2.22                     | 0.53              |
| 3:D:69:GLU:HG3   | 3:D:70:GLY:H      | 1.73                     | 0.53              |
| 3:D:800:LYS:HE3  | 3:D:826:PRO:HD2   | 1.90                     | 0.53              |
| 3:D:828:LYS:H    | 3:D:828:LYS:CD    | 2.22                     | 0.53              |
| 4:E:84:ARG:HG2   | 4:E:88:GLU:HG3    | 1.91                     | 0.53              |
| 5:F:243:ILE:O    | 5:F:247:ILE:HG13  | 2.08                     | 0.53              |
| 5:F:289:GLU:CD   | 5:F:289:GLU:N     | 2.56                     | 0.53              |
| 1:K:11:PHE:HB3   | 1:L:227:ASN:O     | 2.08                     | 0.53              |
| 1:L:52:ALA:HB2   | 1:L:170:VAL:C     | 2.29                     | 0.53              |
| 2:M:258:TYR:O    | 2:M:290:LEU:HD12  | 2.09                     | 0.53              |
| 2:M:512:ARG:CG   | 2:M:523:ILE:HD11  | 2.38                     | 0.53              |
| 2:M:726:ILE:HG13 | 2:M:728:HIS:HB2   | 1.89                     | 0.53              |
| 2:M:759:THR:HB   | 2:M:785:VAL:HG12  | 1.91                     | 0.53              |
| 3:N:1094:LEU:O   | 3:N:1095:THR:C    | 2.47                     | 0.53              |
| 3:N:1121:PRO:CD  | 3:N:1346:ARG:HH21 | 2.21                     | 0.53              |
| 3:N:274:ARG:NE   | 3:N:279:VAL:HG21  | 2.24                     | 0.53              |
| 3:N:387:LEU:N    | 3:N:387:LEU:CD1   | 2.70                     | 0.53              |
| 3:N:458:ALA:O    | 3:N:459:GLU:C     | 2.46                     | 0.53              |
| 3:N:661:MET:HB3  | 3:N:667:ALA:CB    | 2.39                     | 0.53              |
| 3:N:630:VAL:CA   | 3:N:744:GLN:HG2   | 2.37                     | 0.53              |
| 3:N:909:ASN:O    | 3:N:910:SER:C     | 2.46                     | 0.53              |
| 4:O:70:THR:C     | 4:O:72:ARG:H      | 2.11                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:13:VAL:HG22  | 1:A:14:ARG:N      | 2.23                     | 0.53              |
| 1:B:48:ILE:O     | 1:B:148:VAL:HG12  | 2.09                     | 0.53              |
| 2:C:141:HIS:HD2  | 2:C:334:ARG:CG    | 2.21                     | 0.53              |
| 2:C:231:PRO:O    | 2:C:235:LEU:HB2   | 2.07                     | 0.53              |
| 2:C:424:GLY:O    | 2:C:427:VAL:N     | 2.39                     | 0.53              |
| 2:C:712:ALA:O    | 2:C:820:ARG:N     | 2.26                     | 0.53              |
| 2:C:728:HIS:CE1  | 2:C:730:SER:H     | 2.27                     | 0.53              |
| 2:C:730:SER:OG   | 2:C:731:GLU:N     | 2.42                     | 0.53              |
| 2:C:673:LEU:HB2  | 2:C:868:ASP:OD2   | 2.09                     | 0.53              |
| 3:D:1162:GLU:HG3 | 3:D:1162:GLU:O    | 2.08                     | 0.53              |
| 3:D:1479:ASP:HA  | 3:D:1482:ARG:HG3  | 1.89                     | 0.53              |
| 3:D:14:SER:O     | 3:D:15:PRO:C      | 2.47                     | 0.53              |
| 3:D:1500:LYS:C   | 3:D:1502:ALA:N    | 2.61                     | 0.53              |
| 3:D:297:ILE:CD1  | 3:D:298:VAL:HG23  | 2.18                     | 0.53              |
| 3:D:401:TYR:HB2  | 3:D:444:VAL:CG2   | 2.38                     | 0.53              |
| 3:D:481:MET:O    | 3:D:489:ARG:HG3   | 2.07                     | 0.53              |
| 5:F:115:LYS:HB3  | 5:F:119:ILE:HD11  | 1.91                     | 0.53              |
| 5:F:274:THR:HG22 | 5:F:278:LEU:HD11  | 1.90                     | 0.53              |
| 1:K:42:ARG:NH1   | 1:L:31:GLY:O      | 2.42                     | 0.53              |
| 2:M:311:PHE:HA   | 2:M:314:THR:OG1   | 2.08                     | 0.53              |
| 3:N:953:ASP:OD2  | 3:N:1019:PRO:HG2  | 2.09                     | 0.53              |
| 3:N:1293:PHE:CE2 | 3:N:1300:SER:HB3  | 2.44                     | 0.53              |
| 3:N:153:LEU:HD12 | 3:N:157:GLU:OE1   | 2.08                     | 0.53              |
| 3:N:154:THR:HG22 | 3:N:157:GLU:CB    | 2.39                     | 0.53              |
| 3:N:657:LEU:HG   | 3:N:661:MET:HE2   | 1.90                     | 0.53              |
| 3:N:959:GLU:HA   | 3:N:962:GLN:NE2   | 2.23                     | 0.53              |
| 3:N:965:GLU:O    | 3:N:968:ASP:N     | 2.42                     | 0.53              |
| 5:P:102:LEU:CD2  | 5:P:187:LEU:HB2   | 2.39                     | 0.53              |
| 2:C:30:LEU:HD23  | 2:C:44:ILE:HD12   | 1.91                     | 0.53              |
| 2:C:876:VAL:HG13 | 2:C:881:ASN:ND2   | 2.24                     | 0.53              |
| 2:C:958:THR:HG23 | 2:C:961:GLU:HB2   | 1.91                     | 0.53              |
| 3:D:1046:GLN:NE2 | 3:D:1050:GLY:HA2  | 2.23                     | 0.53              |
| 3:D:135:LEU:HD11 | 3:D:148:GLU:HB2   | 1.90                     | 0.53              |
| 3:D:842:VAL:O    | 3:D:842:VAL:HG23  | 2.09                     | 0.53              |
| 1:L:91:ASN:HB3   | 1:L:94:LEU:CD1    | 2.39                     | 0.53              |
| 2:M:157:ARG:HD2  | 2:M:314:THR:HA    | 1.90                     | 0.53              |
| 2:M:141:HIS:HB2  | 2:M:418:LEU:HD22  | 1.91                     | 0.53              |
| 2:M:56:GLU:OE2   | 2:M:356:ARG:HA    | 2.08                     | 0.53              |
| 3:N:1136:LYS:O   | 3:N:1140:ILE:HG13 | 2.09                     | 0.53              |
| 3:N:1347:TYR:CZ  | 3:N:1351:GLU:HG2  | 2.42                     | 0.53              |
| 3:N:168:THR:HG21 | 5:P:93:LEU:CD2    | 2.37                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:191:LEU:HD23  | 3:N:195:VAL:HG12 | 1.90                     | 0.53              |
| 3:N:353:VAL:HG23  | 3:N:353:VAL:O    | 2.09                     | 0.53              |
| 3:N:361:VAL:HA    | 3:N:365:ASP:OD2  | 2.08                     | 0.53              |
| 3:N:212:ARG:HB3   | 3:N:386:HIS:HB2  | 1.91                     | 0.53              |
| 3:N:572:ARG:NH1   | 5:P:84:TYR:N     | 2.57                     | 0.53              |
| 3:N:623:VAL:CG1   | 3:N:624:ASP:H    | 2.21                     | 0.53              |
| 3:N:625:TYR:N     | 3:N:625:TYR:CD1  | 2.77                     | 0.53              |
| 4:O:42:PRO:HG2    | 4:O:43:GLU:H     | 1.74                     | 0.53              |
| 5:P:323:ASP:OD1   | 5:P:325:LYS:HB2  | 2.09                     | 0.53              |
| 1:A:13:VAL:CG2    | 1:A:14:ARG:N     | 2.71                     | 0.53              |
| 1:A:219:ARG:O     | 1:A:222:LEU:N    | 2.42                     | 0.53              |
| 1:B:5:LYS:O       | 1:B:7:LYS:N      | 2.42                     | 0.53              |
| 1:B:97:VAL:CG1    | 1:B:98:THR:H     | 2.19                     | 0.53              |
| 2:C:1058:ASP:OD2  | 2:C:1084:SER:N   | 2.30                     | 0.53              |
| 2:C:41:ASN:HB3    | 2:C:49:ARG:NE    | 2.24                     | 0.53              |
| 2:C:431:HIS:ND1   | 2:C:432:ARG:N    | 2.57                     | 0.53              |
| 2:C:431:HIS:ND1   | 2:C:433:THR:N    | 2.51                     | 0.53              |
| 2:C:545:ASN:HB3   | 2:C:583:LEU:HD11 | 1.90                     | 0.53              |
| 2:C:603:VAL:HG21  | 2:C:643:VAL:HG22 | 1.89                     | 0.53              |
| 2:C:939:ARG:CZ    | 2:C:981:GLU:HG2  | 2.37                     | 0.53              |
| 2:C:93:PRO:HA     | 2:C:117:HIS:HA   | 1.91                     | 0.53              |
| 3:D:1397:LYS:O    | 3:D:1401:GLU:HB2 | 2.09                     | 0.53              |
| 3:D:1405:GLU:O    | 3:D:1412:LYS:CA  | 2.50                     | 0.53              |
| 3:D:1464:GLU:CG   | 3:D:1465:ASN:N   | 2.71                     | 0.53              |
| 3:D:1488:ASP:HA   | 4:E:73:LEU:CD1   | 2.39                     | 0.53              |
| 3:D:204:LEU:HB3   | 3:D:394:LEU:O    | 2.09                     | 0.53              |
| 3:D:686:GLU:HA    | 3:D:689:ASP:OD2  | 2.09                     | 0.53              |
| 3:D:68:PHE:CZ     | 5:F:376:ILE:HG12 | 2.44                     | 0.53              |
| 3:D:703:ASN:ND2   | 3:D:704:ARG:N    | 2.57                     | 0.53              |
| 5:F:110:MET:SD    | 5:F:114:LYS:HE3  | 2.49                     | 0.53              |
| 3:D:564:GLU:HB3   | 5:F:140:ARG:HD2  | 1.90                     | 0.53              |
| 5:F:355:GLU:CA    | 5:F:358:LEU:HB3  | 2.36                     | 0.53              |
| 1:L:94:LEU:O      | 1:L:146:ARG:NH2  | 2.41                     | 0.53              |
| 2:M:1040:LEU:HD23 | 3:N:763:MET:HE3  | 1.89                     | 0.53              |
| 2:M:164:PRO:HD3   | 2:M:266:ARG:CZ   | 2.38                     | 0.53              |
| 2:M:233:GLU:O     | 2:M:237:ARG:HG3  | 2.09                     | 0.53              |
| 2:M:26:TYR:O      | 2:M:29:ALA:HB3   | 2.09                     | 0.53              |
| 2:M:463:GLU:OE2   | 2:M:464:LEU:HG   | 2.09                     | 0.53              |
| 2:M:48:PHE:C      | 2:M:50:GLU:H     | 2.12                     | 0.53              |
| 2:M:835:VAL:HG23  | 2:M:849:VAL:O    | 2.09                     | 0.53              |
| 1:L:30:ARG:HD3    | 2:M:854:PRO:CG   | 2.38                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:961:GLU:O     | 2:M:964:LYS:N     | 2.41                     | 0.53              |
| 3:N:101:HIS:CE1   | 3:N:103:TRP:HB2   | 2.43                     | 0.53              |
| 3:N:108:VAL:HA    | 3:N:109:PRO:C     | 2.29                     | 0.53              |
| 3:N:1106:VAL:CG1  | 3:N:1107:VAL:N    | 2.72                     | 0.53              |
| 3:N:1288:GLU:OE1  | 3:N:1288:GLU:N    | 2.42                     | 0.53              |
| 3:N:1467:ILE:HD11 | 10:N:1528:NE6:C20 | 2.38                     | 0.53              |
| 3:N:287:GLY:C     | 3:N:311:LEU:HD22  | 2.29                     | 0.53              |
| 3:N:341:GLU:OE1   | 3:N:343:LYS:HE3   | 2.09                     | 0.53              |
| 3:N:140:ALA:N     | 3:N:450:TYR:HE2   | 2.06                     | 0.53              |
| 3:N:42:ASP:H      | 3:N:46:ASP:CG     | 2.11                     | 0.53              |
| 3:N:483:HIS:HB2   | 3:N:484:PRO:HD3   | 1.88                     | 0.53              |
| 3:N:511:TRP:N     | 3:N:511:TRP:HE3   | 2.07                     | 0.53              |
| 3:N:709:HIS:HA    | 3:N:1227:GLN:HB3  | 1.90                     | 0.53              |
| 3:N:711:LEU:C     | 3:N:713:ILE:H     | 2.12                     | 0.53              |
| 3:N:87:ARG:HB3    | 3:N:523:ASP:HB2   | 1.90                     | 0.53              |
| 4:O:84:ARG:O      | 4:O:87:LYS:HB3    | 2.09                     | 0.53              |
| 5:P:367:MET:O     | 5:P:368:VAL:C     | 2.47                     | 0.53              |
| 1:A:24:VAL:HG12   | 1:A:25:LEU:N      | 2.23                     | 0.52              |
| 1:B:87:VAL:CG1    | 1:B:122:ILE:HG12  | 2.38                     | 0.52              |
| 2:C:353:ARG:HG2   | 2:C:353:ARG:NH1   | 2.21                     | 0.52              |
| 2:C:602:GLU:HG2   | 2:C:603:VAL:N     | 2.23                     | 0.52              |
| 3:D:1155:VAL:HG12 | 3:D:1156:LEU:N    | 2.24                     | 0.52              |
| 3:D:1114:THR:HB   | 3:D:1195:GLN:CG   | 2.37                     | 0.52              |
| 3:D:12:LEU:HD12   | 3:D:511:TRP:HB2   | 1.91                     | 0.52              |
| 3:D:16:GLU:O      | 3:D:20:SER:N      | 2.42                     | 0.52              |
| 3:D:490:ALA:HA    | 3:D:493:ARG:HE    | 1.74                     | 0.52              |
| 3:D:628:ARG:HG2   | 3:D:629:SER:N     | 2.22                     | 0.52              |
| 5:F:120:THR:HG22  | 5:F:122:LEU:HG    | 1.91                     | 0.52              |
| 3:D:569:ASN:ND2   | 5:F:214:GLN:NE2   | 2.57                     | 0.52              |
| 1:K:73:GLU:CD     | 1:K:130:ALA:HA    | 2.29                     | 0.52              |
| 1:L:176:ARG:HB3   | 1:L:200:TRP:CD1   | 2.44                     | 0.52              |
| 1:L:36:LEU:C      | 1:L:39:PRO:HD2    | 2.29                     | 0.52              |
| 2:M:18:LEU:O      | 2:M:20:GLU:N      | 2.41                     | 0.52              |
| 2:M:218:VAL:CG1   | 2:M:222:MET:HE2   | 2.38                     | 0.52              |
| 2:M:232:GLU:HA    | 2:M:235:LEU:CD1   | 2.37                     | 0.52              |
| 3:N:1112:CYS:HB3  | 3:N:1201:CYS:HB3  | 1.89                     | 0.52              |
| 3:N:1286:THR:CG2  | 3:N:1289:LYS:H    | 2.22                     | 0.52              |
| 3:N:1336:LEU:O    | 3:N:1340:GLY:N    | 2.42                     | 0.52              |
| 3:N:1381:VAL:CG1  | 3:N:1391:GLU:HB2  | 2.39                     | 0.52              |
| 3:N:148:GLU:O     | 3:N:149:LYS:C     | 2.46                     | 0.52              |
| 3:N:466:LYS:HG2   | 3:N:510:GLU:HG2   | 1.91                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:535:PHE:CD1   | 3:N:535:PHE:N     | 2.77                     | 0.52              |
| 2:M:874:LEU:HD21  | 3:N:787:LEU:HD22  | 1.91                     | 0.52              |
| 3:N:852:ALA:O     | 3:N:855:HIS:N     | 2.41                     | 0.52              |
| 3:N:970:LYS:HE2   | 3:N:974:ILE:CG1   | 2.39                     | 0.52              |
| 5:P:154:LYS:O     | 5:P:156:VAL:N     | 2.42                     | 0.52              |
| 5:P:305:GLU:O     | 5:P:309:LYS:HG3   | 2.09                     | 0.52              |
| 1:A:30:ARG:HG3    | 2:C:938:LYS:HZ3   | 1.74                     | 0.52              |
| 1:B:82:LEU:HD23   | 1:B:82:LEU:N      | 2.23                     | 0.52              |
| 2:C:1040:LEU:HD12 | 2:C:1049:LEU:HD13 | 1.90                     | 0.52              |
| 2:C:1101:THR:C    | 2:C:1102:LEU:HD23 | 2.30                     | 0.52              |
| 2:C:649:VAL:CG1   | 2:C:653:ASP:CB    | 2.87                     | 0.52              |
| 2:C:724:ARG:HH21  | 2:C:734:LEU:HB2   | 1.74                     | 0.52              |
| 3:D:1091:SER:C    | 3:D:1093:TYR:N    | 2.58                     | 0.52              |
| 3:D:207:PHE:O     | 3:D:391:ALA:N     | 2.42                     | 0.52              |
| 3:D:302:GLN:O     | 3:D:304:LEU:N     | 2.41                     | 0.52              |
| 3:D:351:MET:CG    | 3:D:370:ALA:HB2   | 2.38                     | 0.52              |
| 3:D:520:LEU:HD21  | 3:D:524:LEU:CB    | 2.39                     | 0.52              |
| 3:D:556:LYS:O     | 3:D:559:ALA:HB3   | 2.08                     | 0.52              |
| 3:D:807:ALA:HB2   | 3:D:833:GLU:CD    | 2.29                     | 0.52              |
| 3:D:989:TYR:CA    | 3:D:992:ILE:HD12  | 2.37                     | 0.52              |
| 5:F:265:VAL:O     | 5:F:266:GLU:C     | 2.46                     | 0.52              |
| 5:F:308:LEU:CD2   | 5:F:308:LEU:H     | 2.20                     | 0.52              |
| 3:D:534:ARG:NH2   | 5:F:314:PRO:O     | 2.43                     | 0.52              |
| 1:K:112:ARG:HE    | 1:K:125:PRO:HB2   | 1.74                     | 0.52              |
| 1:K:1:MET:N       | 1:K:6:LEU:HD13    | 2.20                     | 0.52              |
| 2:M:1095:LEU:O    | 2:M:1096:ALA:HB3  | 2.09                     | 0.52              |
| 2:M:334:ARG:HH11  | 2:M:418:LEU:HD11  | 1.74                     | 0.52              |
| 2:M:918:LEU:HD13  | 2:M:967:PHE:O     | 2.10                     | 0.52              |
| 3:N:1117:TYR:CD1  | 3:N:1118:ILE:N    | 2.77                     | 0.52              |
| 3:N:181:ASP:C     | 3:N:183:GLU:N     | 2.62                     | 0.52              |
| 3:N:225:LEU:HD12  | 3:N:333:LEU:HD11  | 1.91                     | 0.52              |
| 3:N:212:ARG:HD3   | 3:N:342:PRO:HB2   | 1.89                     | 0.52              |
| 3:N:477:LEU:HD11  | 3:N:495:ARG:HD3   | 1.90                     | 0.52              |
| 3:N:59:ALA:C      | 3:N:61:GLY:H      | 2.12                     | 0.52              |
| 3:N:627:GLY:HA3   | 3:N:648:MET:HE2   | 1.91                     | 0.52              |
| 3:N:844:ALA:N     | 3:N:848:GLU:OE1   | 2.42                     | 0.52              |
| 1:A:109:VAL:CG1   | 1:A:129:ILE:HB    | 2.39                     | 0.52              |
| 1:B:71:VAL:HG13   | 1:B:132:LEU:HD23  | 1.90                     | 0.52              |
| 2:C:1000:MET:HB2  | 2:C:1003:ASP:HB2  | 1.91                     | 0.52              |
| 2:C:18:LEU:O      | 2:C:20:GLU:N      | 2.42                     | 0.52              |
| 2:C:200:LEU:HD22  | 2:C:300:ASP:CB    | 2.39                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:631:SER:O    | 2:C:634:GLY:N     | 2.36                     | 0.52              |
| 2:C:776:SER:CB   | 2:C:780:GLU:HB2   | 2.39                     | 0.52              |
| 3:D:1016:PRO:HA  | 3:D:1021:TYR:HD1  | 1.70                     | 0.52              |
| 3:D:1381:VAL:CG2 | 3:D:1382:THR:N    | 2.72                     | 0.52              |
| 3:D:252:ARG:NH2  | 3:D:300:LYS:HG2   | 2.24                     | 0.52              |
| 3:D:30:GLU:HB3   | 3:D:40:GLU:CB     | 2.39                     | 0.52              |
| 3:D:760:ARG:HH12 | 4:E:61:GLU:HB2    | 1.74                     | 0.52              |
| 3:D:536:ALA:HB1  | 5:F:317:LEU:HD23  | 1.91                     | 0.52              |
| 5:F:348:SER:O    | 5:F:352:GLU:HG3   | 2.09                     | 0.52              |
| 2:M:918:LEU:HD12 | 2:M:968:LEU:O     | 2.10                     | 0.52              |
| 3:N:133:ILE:HB   | 3:N:454:ALA:CB    | 2.30                     | 0.52              |
| 3:N:1491:THR:C   | 3:N:1493:LYS:N    | 2.63                     | 0.52              |
| 3:N:238:PRO:HD3  | 3:N:318:ARG:HA    | 1.91                     | 0.52              |
| 3:N:410:SER:O    | 3:N:413:ASP:OD2   | 2.27                     | 0.52              |
| 5:P:265:VAL:HG12 | 5:P:269:ASN:HD21  | 1.74                     | 0.52              |
| 5:P:93:LEU:O     | 5:P:95:THR:N      | 2.42                     | 0.52              |
| 1:B:137:ARG:HG2  | 1:B:137:ARG:NH1   | 2.24                     | 0.52              |
| 2:C:288:ARG:HG3  | 2:C:289:THR:N     | 2.24                     | 0.52              |
| 2:C:517:ARG:O    | 2:C:518:LYS:HG2   | 2.09                     | 0.52              |
| 2:C:778:PHE:CE2  | 5:F:419:ARG:NH1   | 2.78                     | 0.52              |
| 2:C:806:LEU:HD22 | 2:C:813:VAL:HG22  | 1.91                     | 0.52              |
| 3:D:1103:HIS:HB2 | 3:D:1223:ILE:HD11 | 1.90                     | 0.52              |
| 3:D:14:SER:CB    | 3:D:17:LYS:H      | 2.20                     | 0.52              |
| 3:D:379:ALA:O    | 3:D:380:GLU:HG3   | 2.10                     | 0.52              |
| 3:D:643:GLY:HA3  | 3:D:727:GLN:HB2   | 1.91                     | 0.52              |
| 3:D:811:GLU:O    | 3:D:816:HIS:N     | 2.40                     | 0.52              |
| 3:D:826:PRO:HD2  | 3:D:829:VAL:CG2   | 2.40                     | 0.52              |
| 4:E:70:THR:C     | 4:E:72:ARG:N      | 2.63                     | 0.52              |
| 2:M:1030:GLN:HG2 | 3:N:626:SER:HB2   | 1.92                     | 0.52              |
| 2:M:1114:GLY:C   | 2:M:1116:ALA:H    | 2.12                     | 0.52              |
| 2:M:310:LEU:CD1  | 2:M:314:THR:HG23  | 2.40                     | 0.52              |
| 2:M:499:ALA:HB2  | 2:M:533:ASP:HB2   | 1.90                     | 0.52              |
| 2:M:68:PHE:CZ    | 2:M:71:TYR:N      | 2.77                     | 0.52              |
| 2:M:720:GLU:C    | 2:M:721:ARG:HG3   | 2.29                     | 0.52              |
| 2:M:970:GLY:O    | 2:M:988:VAL:HA    | 2.10                     | 0.52              |
| 3:N:1251:ASP:O   | 3:N:1270:ALA:HB2  | 2.10                     | 0.52              |
| 3:N:181:ASP:O    | 3:N:183:GLU:N     | 2.35                     | 0.52              |
| 3:N:249:TYR:CE1  | 3:N:330:THR:CG2   | 2.92                     | 0.52              |
| 3:N:24:GLY:HA3   | 3:N:49:ILE:HG23   | 1.91                     | 0.52              |
| 3:N:654:LYS:O    | 3:N:657:LEU:HB3   | 2.09                     | 0.52              |
| 4:O:37:ASN:HA    | 4:O:93:TYR:CE2    | 2.43                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:P:110:MET:HE2  | 5:P:111:GLU:HG3  | 1.92                     | 0.52              |
| 5:P:242:TRP:O    | 5:P:245:GLN:HG2  | 2.10                     | 0.52              |
| 1:A:178:ALA:CB   | 2:C:864:GLY:HA3  | 2.39                     | 0.52              |
| 1:A:16:GLN:NE2   | 1:B:235:ALA:HB1  | 2.25                     | 0.52              |
| 1:B:73:GLU:HG3   | 1:B:130:ALA:CB   | 2.39                     | 0.52              |
| 2:C:211:LEU:C    | 2:C:213:ALA:N    | 2.59                     | 0.52              |
| 2:C:240:THR:C    | 2:C:242:LEU:H    | 2.12                     | 0.52              |
| 2:C:31:GLN:CA    | 2:C:35:PRO:HG2   | 2.39                     | 0.52              |
| 3:D:1117:TYR:HD1 | 3:D:1118:ILE:N   | 2.08                     | 0.52              |
| 3:D:137:PRO:HG2  | 3:D:138:LYS:H    | 1.74                     | 0.52              |
| 3:D:1403:LEU:C   | 3:D:1405:GLU:N   | 2.63                     | 0.52              |
| 3:D:152:LEU:HD12 | 3:D:153:LEU:H    | 1.73                     | 0.52              |
| 3:D:207:PHE:HB2  | 3:D:391:ALA:CB   | 2.37                     | 0.52              |
| 3:D:226:PRO:CB   | 3:D:231:VAL:HG21 | 2.40                     | 0.52              |
| 3:D:456:MET:SD   | 3:D:568:ARG:HD3  | 2.49                     | 0.52              |
| 2:C:1031:ARG:CA  | 3:D:622:ARG:HH12 | 2.22                     | 0.52              |
| 3:D:703:ASN:HD22 | 3:D:704:ARG:N    | 2.07                     | 0.52              |
| 3:D:771:SER:O    | 3:D:775:GLY:N    | 2.42                     | 0.52              |
| 2:C:1015:LEU:CD1 | 5:F:335:ASP:HA   | 2.39                     | 0.52              |
| 1:K:98:THR:HG21  | 1:K:141:GLU:HB3  | 1.92                     | 0.52              |
| 1:K:24:VAL:HG22  | 1:K:196:THR:HG23 | 1.91                     | 0.52              |
| 1:K:76:VAL:O     | 1:K:80:LEU:HG    | 2.10                     | 0.52              |
| 1:K:86:VAL:HG12  | 1:K:124:ASN:CG   | 2.29                     | 0.52              |
| 2:M:1034:GLU:O   | 2:M:1035:MET:C   | 2.48                     | 0.52              |
| 2:M:1085:PHE:O   | 2:M:1086:ARG:C   | 2.48                     | 0.52              |
| 2:M:401:LEU:O    | 2:M:404:LEU:HB3  | 2.10                     | 0.52              |
| 2:M:419:THR:CG2  | 2:M:420:ARG:N    | 2.72                     | 0.52              |
| 2:M:511:GLU:O    | 2:M:526:PRO:HD3  | 2.10                     | 0.52              |
| 2:M:810:ASP:N    | 2:M:811:PRO:CD   | 2.73                     | 0.52              |
| 3:N:1435:LEU:O   | 3:N:1436:SER:C   | 2.47                     | 0.52              |
| 3:N:322:VAL:CG2  | 3:N:333:LEU:HD22 | 2.40                     | 0.52              |
| 3:N:520:LEU:O    | 3:N:525:ARG:NH1  | 2.43                     | 0.52              |
| 3:N:587:ARG:HB3  | 3:N:587:ARG:CZ   | 2.39                     | 0.52              |
| 3:N:602:SER:H    | 3:N:605:ASP:CG   | 2.11                     | 0.52              |
| 3:N:674:ARG:HG3  | 3:N:674:ARG:NH1  | 2.24                     | 0.52              |
| 3:N:985:ASP:OD2  | 3:N:985:ASP:N    | 2.42                     | 0.52              |
| 4:O:40:LEU:HD12  | 4:O:41:GLU:H     | 1.74                     | 0.52              |
| 5:P:152:ASP:HA   | 5:P:156:VAL:CG1  | 2.39                     | 0.52              |
| 5:P:253:ASP:CA   | 5:P:259:ARG:HH12 | 2.20                     | 0.52              |
| 5:P:355:GLU:C    | 5:P:358:LEU:HB3  | 2.30                     | 0.52              |
| 1:A:34:VAL:C     | 1:A:36:LEU:N     | 2.63                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:38:ASN:HB2    | 11:B:702:HOH:O    | 2.09                     | 0.52              |
| 2:C:543:ASN:HB2   | 2:C:565:GLN:NE2   | 2.25                     | 0.52              |
| 3:D:1098:LEU:H    | 3:D:1098:LEU:HD12 | 1.75                     | 0.52              |
| 3:D:1167:SER:HB3  | 3:D:1170:ASP:OD2  | 2.09                     | 0.52              |
| 3:D:1381:VAL:HG22 | 3:D:1382:THR:N    | 2.24                     | 0.52              |
| 3:D:1400:VAL:HB   | 3:D:1401:GLU:OE1  | 2.09                     | 0.52              |
| 3:D:1485:GLN:OE1  | 4:E:79:LEU:N      | 2.41                     | 0.52              |
| 3:D:164:GLY:HA3   | 3:D:447:VAL:CG1   | 2.40                     | 0.52              |
| 3:D:219:GLU:HG2   | 3:D:220:ARG:N     | 2.23                     | 0.52              |
| 3:D:28:LYS:O      | 3:D:43:GLY:HA2    | 2.10                     | 0.52              |
| 3:D:227:LEU:HG    | 3:D:326:GLU:CD    | 2.30                     | 0.52              |
| 3:D:406:ASP:HB2   | 3:D:423:ASP:CA    | 2.40                     | 0.52              |
| 3:D:411:THR:HA    | 3:D:435:VAL:CG1   | 2.36                     | 0.52              |
| 3:D:662:GLU:HA    | 3:D:667:ALA:O     | 2.09                     | 0.52              |
| 4:E:39:VAL:HG11   | 4:E:72:ARG:HB3    | 1.91                     | 0.52              |
| 5:F:291:ILE:O     | 5:F:292:ALA:C     | 2.47                     | 0.52              |
| 5:F:382:THR:CG2   | 5:F:394:ARG:HB2   | 2.39                     | 0.52              |
| 5:F:417:LYS:C     | 5:F:419:ARG:N     | 2.63                     | 0.52              |
| 1:K:209:GLU:HA    | 1:K:212:ASN:ND2   | 2.25                     | 0.52              |
| 1:L:175:ARG:N     | 1:L:200:TRP:O     | 2.42                     | 0.52              |
| 2:M:95:TYR:HA     | 2:M:113:VAL:C     | 2.29                     | 0.52              |
| 2:M:166:PRO:HB2   | 2:M:169:GLY:HA3   | 1.91                     | 0.52              |
| 2:M:157:ARG:CD    | 2:M:314:THR:HG22  | 2.35                     | 0.52              |
| 2:M:102:HIS:CG    | 2:M:365:ASP:OD1   | 2.63                     | 0.52              |
| 2:M:513:VAL:N     | 2:M:524:VAL:O     | 2.42                     | 0.52              |
| 2:M:691:SER:O     | 2:M:693:GLU:N     | 2.43                     | 0.52              |
| 3:N:1442:ASN:HD21 | 3:N:1445:HIS:HB2  | 1.75                     | 0.52              |
| 3:N:219:GLU:CG    | 3:N:220:ARG:H     | 2.12                     | 0.52              |
| 3:N:525:ARG:N     | 3:N:526:PRO:CD    | 2.69                     | 0.52              |
| 3:N:552:ASN:O     | 3:N:555:LYS:HB2   | 2.09                     | 0.52              |
| 3:N:662:GLU:HG2   | 3:N:663:GLU:N     | 2.25                     | 0.52              |
| 3:N:674:ARG:HG3   | 3:N:674:ARG:HH11  | 1.74                     | 0.52              |
| 2:M:1039:ALA:CB   | 3:N:713:ILE:HD12  | 2.39                     | 0.52              |
| 5:P:117:SER:CB    | 5:P:124:PRO:HG3   | 2.40                     | 0.52              |
| 5:P:367:MET:HA    | 5:P:370:LYS:HG2   | 1.91                     | 0.52              |
| 1:B:76:VAL:O      | 1:B:79:ILE:HB     | 2.10                     | 0.52              |
| 2:C:1102:LEU:HD23 | 2:C:1108:PRO:HA   | 1.91                     | 0.52              |
| 2:C:1090:LYS:HE2  | 2:C:1112:PHE:CZ   | 2.45                     | 0.52              |
| 2:C:180:GLY:HA2   | 2:C:223:ASP:CG    | 2.30                     | 0.52              |
| 2:C:23:VAL:HA     | 2:C:121:MET:HE3   | 1.86                     | 0.52              |
| 2:C:285:LEU:HD11  | 2:C:288:ARG:C     | 2.30                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:41:ASN:O      | 2:C:46:ALA:HB2    | 2.09                     | 0.52              |
| 3:D:1047:LYS:HG2  | 3:D:1053:PHE:CZ   | 2.44                     | 0.52              |
| 3:D:1165:TYR:CE2  | 3:D:1206:GLY:HA2  | 2.45                     | 0.52              |
| 3:D:1381:VAL:HG13 | 3:D:1389:LEU:O    | 2.10                     | 0.52              |
| 3:D:1479:ASP:CA   | 3:D:1482:ARG:HG3  | 2.40                     | 0.52              |
| 3:D:1491:THR:O    | 3:D:1494:ALA:HB3  | 2.10                     | 0.52              |
| 3:D:566:ILE:O     | 3:D:570:GLU:N     | 2.37                     | 0.52              |
| 3:D:567:ILE:O     | 3:D:570:GLU:HB3   | 2.09                     | 0.52              |
| 3:D:607:LEU:HG    | 3:D:608:SER:N     | 2.24                     | 0.52              |
| 3:D:665:GLY:O     | 3:D:667:ALA:N     | 2.43                     | 0.52              |
| 3:D:798:GLU:CG    | 3:D:799:LYS:N     | 2.73                     | 0.52              |
| 3:D:82:LYS:HB3    | 3:D:84:ILE:HG22   | 1.92                     | 0.52              |
| 3:D:970:LYS:O     | 3:D:973:GLN:HB2   | 2.09                     | 0.52              |
| 4:E:26:ARG:O      | 4:E:30:LEU:CB     | 2.58                     | 0.52              |
| 5:F:235:PHE:O     | 5:F:236:SER:C     | 2.47                     | 0.52              |
| 5:F:319:THR:O     | 5:F:328:PHE:HA    | 2.10                     | 0.52              |
| 1:K:74:ASP:O      | 1:K:78:ILE:HG13   | 2.10                     | 0.52              |
| 2:M:104:ASP:N     | 2:M:104:ASP:OD1   | 2.42                     | 0.52              |
| 2:M:193:LEU:O     | 2:M:196:LEU:HG    | 2.08                     | 0.52              |
| 2:M:228:ALA:C     | 2:M:229:MET:HG3   | 2.30                     | 0.52              |
| 2:M:263:ASP:HB2   | 2:M:264:PRO:HD3   | 1.91                     | 0.52              |
| 2:M:421:GLU:HG2   | 2:M:421:GLU:O     | 2.09                     | 0.52              |
| 2:M:6:PHE:HB2     | 2:M:902:ILE:O     | 2.09                     | 0.52              |
| 2:M:799:ILE:O     | 2:M:799:ILE:HG13  | 2.09                     | 0.52              |
| 2:M:816:LYS:HD2   | 2:M:816:LYS:H     | 1.73                     | 0.52              |
| 2:M:854:PRO:O     | 2:M:856:GLU:N     | 2.42                     | 0.52              |
| 2:M:863:ASP:OD2   | 2:M:865:THR:HG23  | 2.09                     | 0.52              |
| 3:N:1102:THR:HB   | 3:N:1105:ILE:HD12 | 1.91                     | 0.52              |
| 3:N:129:PHE:O     | 3:N:130:SER:HB2   | 2.10                     | 0.52              |
| 3:N:86:ARG:NH1    | 3:N:522:PRO:HB2   | 2.24                     | 0.52              |
| 3:N:90:MET:HE2    | 3:N:519:VAL:O     | 2.09                     | 0.52              |
| 5:P:211:ASP:O     | 5:P:215:GLU:HG2   | 2.10                     | 0.52              |
| 2:C:649:VAL:HG13  | 2:C:653:ASP:CG    | 2.29                     | 0.52              |
| 2:C:727:PRO:HG2   | 2:C:785:VAL:O     | 2.10                     | 0.52              |
| 2:C:857:ASP:HB3   | 2:C:978:ARG:HG2   | 1.92                     | 0.52              |
| 2:C:676:ILE:CG1   | 2:C:873:PRO:HG3   | 2.40                     | 0.52              |
| 2:C:885:ILE:HG22  | 2:C:886:LEU:N     | 2.25                     | 0.52              |
| 3:D:1379:VAL:O    | 3:D:1392:GLY:HA2  | 2.09                     | 0.52              |
| 3:D:1483:PHE:O    | 3:D:1484:THR:C    | 2.48                     | 0.52              |
| 3:D:1497:GLU:O    | 3:D:1501:GLU:HB2  | 2.10                     | 0.52              |
| 3:D:412:GLY:N     | 3:D:435:VAL:HB    | 2.22                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:560:GLN:O    | 3:D:561:GLY:C    | 2.45                     | 0.52              |
| 3:D:729:HIS:HD2  | 3:D:731:LEU:H    | 1.58                     | 0.52              |
| 3:D:631:ILE:CG2  | 3:D:745:MET:HG3  | 2.32                     | 0.52              |
| 3:D:945:SER:OG   | 3:D:947:ILE:CG2  | 2.57                     | 0.52              |
| 3:D:966:GLU:O    | 3:D:969:ARG:HG2  | 2.09                     | 0.52              |
| 5:F:132:ARG:HB3  | 5:F:136:LEU:CD1  | 2.40                     | 0.52              |
| 5:F:288:TYR:O    | 5:F:292:ALA:N    | 2.32                     | 0.52              |
| 1:L:104:GLU:HB3  | 1:L:137:ARG:CG   | 2.28                     | 0.52              |
| 2:M:112:GLU:OE1  | 2:M:112:GLU:HA   | 2.09                     | 0.52              |
| 2:M:141:HIS:HE1  | 2:M:144:PRO:HD3  | 1.74                     | 0.52              |
| 2:M:606:VAL:HG12 | 2:M:611:ILE:HG12 | 1.92                     | 0.52              |
| 2:M:802:ARG:HG2  | 2:M:803:THR:N    | 2.24                     | 0.52              |
| 3:N:1147:ARG:HB2 | 3:N:1166:LEU:CD1 | 2.36                     | 0.52              |
| 3:N:1152:GLU:HG2 | 3:N:1153:VAL:N   | 2.25                     | 0.52              |
| 3:N:1208:ASP:OD1 | 3:N:1210:SER:N   | 2.32                     | 0.52              |
| 3:N:1296:SER:O   | 3:N:1298:GLY:N   | 2.43                     | 0.52              |
| 3:N:1304:LYS:HG2 | 3:N:1305:LEU:N   | 2.24                     | 0.52              |
| 3:N:1401:GLU:OE1 | 3:N:1401:GLU:N   | 2.42                     | 0.52              |
| 3:N:266:GLU:OE2  | 3:N:315:ARG:NH1  | 2.41                     | 0.52              |
| 3:N:584:ASN:OD1  | 3:N:590:PRO:CD   | 2.47                     | 0.52              |
| 3:N:638:LYS:O    | 3:N:640:HIS:N    | 2.43                     | 0.52              |
| 3:N:711:LEU:HD23 | 3:N:735:ALA:HB2  | 1.92                     | 0.52              |
| 5:P:224:VAL:O    | 5:P:225:GLU:C    | 2.48                     | 0.52              |
| 1:A:229:GLN:O    | 1:B:13:VAL:N     | 2.43                     | 0.52              |
| 1:B:26:GLU:OE1   | 1:B:194:LYS:HG3  | 2.10                     | 0.52              |
| 2:C:250:ARG:HB3  | 2:C:253:ALA:HB2  | 1.92                     | 0.52              |
| 2:C:300:ASP:C    | 2:C:302:VAL:H    | 2.14                     | 0.52              |
| 2:C:472:ARG:NH2  | 2:C:479:VAL:HG12 | 2.25                     | 0.52              |
| 2:C:520:GLU:HA   | 2:C:520:GLU:OE1  | 2.08                     | 0.52              |
| 3:D:1380:GLU:O   | 3:D:1417:TRP:HB2 | 2.10                     | 0.52              |
| 3:D:166:GLN:HA   | 3:D:395:VAL:O    | 2.10                     | 0.52              |
| 3:D:259:VAL:O    | 3:D:260:GLU:HG3  | 2.10                     | 0.52              |
| 3:D:241:ILE:HD11 | 3:D:310:LEU:HD22 | 1.91                     | 0.52              |
| 3:D:800:LYS:CE   | 3:D:826:PRO:HD3  | 2.39                     | 0.52              |
| 5:F:117:SER:CB   | 5:F:124:PRO:HG3  | 2.40                     | 0.52              |
| 1:L:216:GLU:O    | 1:L:217:ILE:C    | 2.48                     | 0.52              |
| 2:M:1056:LYS:HD3 | 3:N:623:VAL:CG1  | 2.35                     | 0.52              |
| 2:M:202:TYR:HB2  | 2:M:207:LEU:HD21 | 1.92                     | 0.52              |
| 2:M:157:ARG:HH11 | 2:M:314:THR:HA   | 1.74                     | 0.52              |
| 2:M:311:PHE:HA   | 2:M:314:THR:HG1  | 1.74                     | 0.52              |
| 2:M:789:SER:HB2  | 2:M:791:ARG:HE   | 1.75                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1336:LEU:HD12 | 3:N:1340:GLY:C    | 2.31                     | 0.52              |
| 3:N:142:LEU:HB2   | 3:N:145:VAL:O     | 2.10                     | 0.52              |
| 3:N:1467:ILE:HD11 | 10:N:1528:NE6:C19 | 2.40                     | 0.52              |
| 3:N:355:VAL:CG1   | 3:N:359:ALA:HB3   | 2.40                     | 0.52              |
| 3:N:409:VAL:CG1   | 3:N:413:ASP:OD2   | 2.57                     | 0.52              |
| 3:N:527:MET:HA    | 3:N:537:THR:HG22  | 1.91                     | 0.52              |
| 3:N:909:ASN:HA    | 3:N:912:LYS:NZ    | 2.25                     | 0.52              |
| 3:N:951:ILE:HG23  | 3:N:952:ASP:N     | 2.25                     | 0.52              |
| 3:N:988:ARG:O     | 3:N:989:TYR:C     | 2.47                     | 0.52              |
| 5:P:256:ARG:HG2   | 5:P:256:ARG:HH11  | 1.75                     | 0.52              |
| 5:P:353:GLU:CG    | 5:P:417:LYS:HD3   | 2.40                     | 0.52              |
| 5:P:351:SER:HA    | 5:P:354:LEU:HD12  | 1.91                     | 0.52              |
| 5:P:353:GLU:HG3   | 5:P:356:LYS:HD2   | 1.92                     | 0.52              |
| 1:A:50:GLY:N      | 1:A:147:GLY:O     | 2.42                     | 0.52              |
| 1:A:36:LEU:O      | 1:A:39:PRO:HD2    | 2.09                     | 0.52              |
| 1:A:81:ASN:HD22   | 1:A:81:ASN:N      | 2.08                     | 0.52              |
| 1:A:88:ARG:HG3    | 1:A:204:SER:O     | 2.10                     | 0.52              |
| 2:C:674:VAL:HA    | 2:C:869:VAL:O     | 2.09                     | 0.52              |
| 2:C:572:ILE:HD11  | 2:C:701:THR:HB    | 1.92                     | 0.52              |
| 3:D:998:GLU:O     | 3:D:1001:GLU:HB3  | 2.09                     | 0.52              |
| 3:D:135:LEU:CD2   | 3:D:135:LEU:N     | 2.64                     | 0.52              |
| 3:D:348:GLN:HB2   | 3:D:351:MET:SD    | 2.50                     | 0.52              |
| 3:D:443:VAL:HG12  | 3:D:444:VAL:N     | 2.25                     | 0.52              |
| 3:D:527:MET:SD    | 3:D:537:THR:CG2   | 2.98                     | 0.52              |
| 3:D:953:ASP:C     | 3:D:955:VAL:H     | 2.12                     | 0.52              |
| 4:E:80:VAL:HB     | 4:E:81:PRO:CD     | 2.39                     | 0.52              |
| 3:D:560:GLN:C     | 5:F:132:ARG:NH1   | 2.64                     | 0.52              |
| 5:F:79:ASP:O      | 5:F:80:PRO:C      | 2.46                     | 0.52              |
| 1:L:61:VAL:CG2    | 1:L:163:ASN:HB3   | 2.39                     | 0.52              |
| 2:M:108:ILE:CG2   | 2:M:368:THR:HG21  | 2.40                     | 0.52              |
| 2:M:373:VAL:CG1   | 2:M:374:ASN:H     | 2.18                     | 0.52              |
| 2:M:514:VAL:O     | 2:M:514:VAL:HG23  | 2.10                     | 0.52              |
| 2:M:640:ARG:O     | 2:M:656:ALA:HA    | 2.09                     | 0.52              |
| 2:M:715:THR:HG22  | 2:M:717:LEU:N     | 2.23                     | 0.52              |
| 2:M:807:ARG:C     | 2:M:809:GLY:H     | 2.12                     | 0.52              |
| 1:K:178:ALA:HB2   | 2:M:864:GLY:CA    | 2.40                     | 0.52              |
| 2:M:907:ASP:CG    | 2:M:908:GLY:H     | 2.12                     | 0.52              |
| 3:N:1118:ILE:HG23 | 3:N:1190:SER:HB3  | 1.91                     | 0.52              |
| 3:N:1299:PHE:N    | 3:N:1299:PHE:CD1  | 2.77                     | 0.52              |
| 3:N:177:ALA:HB3   | 3:N:191:LEU:O     | 2.09                     | 0.52              |
| 3:N:484:PRO:O     | 3:N:489:ARG:CB    | 2.51                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:664:LYS:O     | 3:N:666:ILE:HG12  | 2.09                     | 0.52              |
| 3:N:787:LEU:O     | 3:N:788:GLY:C     | 2.48                     | 0.52              |
| 3:N:851:LEU:O     | 3:N:854:ALA:HB3   | 2.10                     | 0.52              |
| 3:N:937:TYR:H     | 3:N:937:TYR:HD1   | 1.56                     | 0.52              |
| 5:P:145:PRO:CB    | 5:P:150:THR:H     | 2.23                     | 0.52              |
| 5:P:279:GLN:HA    | 5:P:284:ARG:O     | 2.10                     | 0.52              |
| 5:P:380:GLU:HA    | 5:P:385:GLU:OE1   | 2.10                     | 0.52              |
| 1:B:32:PHE:HA     | 1:B:35:THR:OG1    | 2.10                     | 0.51              |
| 2:C:277:ALA:O     | 2:C:281:LEU:N     | 2.43                     | 0.51              |
| 2:C:282:GLY:O     | 2:C:283:ILE:HD13  | 2.09                     | 0.51              |
| 2:C:480:THR:HG22  | 2:C:482:GLU:H     | 1.73                     | 0.51              |
| 2:C:580:MET:HB3   | 2:C:584:GLU:CD    | 2.29                     | 0.51              |
| 2:C:589:ARG:HA    | 2:C:596:TYR:OH    | 2.10                     | 0.51              |
| 2:C:713:ARG:H     | 2:C:720:GLU:CD    | 2.13                     | 0.51              |
| 3:D:104:PHE:O     | 3:D:112:ILE:HG12  | 2.10                     | 0.51              |
| 3:D:1295:GLU:HG2  | 3:D:1300:SER:OG   | 2.09                     | 0.51              |
| 3:D:1378:TYR:OH   | 3:D:1431:THR:HA   | 2.09                     | 0.51              |
| 3:D:1099:VAL:HG12 | 10:D:1529:NE6:H14 | 1.91                     | 0.51              |
| 3:D:209:ARG:O     | 3:D:347:VAL:N     | 2.39                     | 0.51              |
| 3:D:324:ALA:HB1   | 3:D:331:VAL:HG11  | 1.91                     | 0.51              |
| 5:F:169:GLU:CD    | 5:F:169:GLU:H     | 2.12                     | 0.51              |
| 5:F:378:GLY:HA3   | 5:F:381:HIS:NE2   | 2.24                     | 0.51              |
| 5:F:381:HIS:O     | 5:F:384:GLU:N     | 2.37                     | 0.51              |
| 2:M:122:THR:HG22  | 2:M:123:GLU:H     | 1.74                     | 0.51              |
| 2:M:202:TYR:HB2   | 2:M:207:LEU:HD11  | 1.92                     | 0.51              |
| 2:M:267:TYR:CD2   | 2:M:271:GLU:HB2   | 2.45                     | 0.51              |
| 2:M:193:LEU:HD11  | 2:M:303:PHE:CD2   | 2.45                     | 0.51              |
| 2:M:526:PRO:O     | 2:M:529:VAL:HG23  | 2.10                     | 0.51              |
| 2:M:759:THR:HB    | 2:M:785:VAL:HG11  | 1.92                     | 0.51              |
| 2:M:8:ARG:HH11    | 2:M:8:ARG:HG3     | 1.76                     | 0.51              |
| 2:M:554:ASP:HA    | 3:N:1061:PHE:CZ   | 2.45                     | 0.51              |
| 3:N:1428:ALA:C    | 3:N:1430:SER:H    | 2.14                     | 0.51              |
| 3:N:22:SER:OG     | 3:N:92:HIS:ND1    | 2.42                     | 0.51              |
| 3:N:465:LEU:HD13  | 3:N:509:PRO:O     | 2.09                     | 0.51              |
| 3:N:558:LEU:C     | 3:N:560:GLN:N     | 2.62                     | 0.51              |
| 3:N:566:ILE:CA    | 3:N:569:ASN:HB3   | 2.40                     | 0.51              |
| 3:N:570:GLU:HB2   | 5:P:214:GLN:NE2   | 2.25                     | 0.51              |
| 3:N:701:LEU:O     | 3:N:747:VAL:HA    | 2.09                     | 0.51              |
| 4:O:26:ARG:O      | 4:O:29:GLN:HG2    | 2.10                     | 0.51              |
| 4:O:86:GLN:O      | 4:O:90:GLU:HG3    | 2.10                     | 0.51              |
| 5:P:368:VAL:O     | 5:P:371:LEU:HB2   | 2.10                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:308:ARG:O    | 2:C:311:PHE:HB2  | 2.10                     | 0.51              |
| 2:C:513:VAL:HG12 | 2:C:514:VAL:N    | 2.24                     | 0.51              |
| 2:C:513:VAL:N    | 2:C:524:VAL:O    | 2.42                     | 0.51              |
| 2:C:54:ILE:HD13  | 2:C:355:VAL:CG1  | 2.39                     | 0.51              |
| 2:C:861:LEU:CB   | 2:C:862:PRO:HD2  | 2.40                     | 0.51              |
| 2:C:689:VAL:HG21 | 2:C:870:ILE:HB   | 1.92                     | 0.51              |
| 2:C:914:ILE:C    | 2:C:916:GLU:N    | 2.62                     | 0.51              |
| 2:C:983:ILE:O    | 2:C:985:GLY:N    | 2.43                     | 0.51              |
| 3:D:1094:LEU:O   | 3:D:1095:THR:C   | 2.49                     | 0.51              |
| 3:D:1103:HIS:HD2 | 3:D:1462:LEU:HB2 | 1.75                     | 0.51              |
| 3:D:1398:TRP:HA  | 3:D:1402:ALA:H   | 1.76                     | 0.51              |
| 3:D:36:THR:C     | 3:D:37:LEU:HG    | 2.31                     | 0.51              |
| 3:D:39:PRO:HG2   | 3:D:53:ILE:HD11  | 1.92                     | 0.51              |
| 3:D:583:ASP:OD2  | 3:D:586:ARG:HG2  | 2.10                     | 0.51              |
| 3:D:900:ILE:HG22 | 3:D:902:LEU:N    | 2.25                     | 0.51              |
| 5:F:135:ILE:HD11 | 5:F:178:ARG:HA   | 1.92                     | 0.51              |
| 5:F:321:ILE:CG2  | 5:F:322:GLY:N    | 2.73                     | 0.51              |
| 5:F:358:LEU:HG   | 5:F:359:SER:N    | 2.25                     | 0.51              |
| 1:L:34:VAL:C     | 1:L:36:LEU:N     | 2.60                     | 0.51              |
| 2:M:1007:ALA:HB2 | 3:N:648:MET:HE2  | 1.92                     | 0.51              |
| 2:M:1072:LYS:C   | 3:N:659:LYS:HE3  | 2.31                     | 0.51              |
| 2:M:263:ASP:HB2  | 2:M:264:PRO:CD   | 2.40                     | 0.51              |
| 2:M:405:ARG:HD2  | 2:M:442:GLU:OE2  | 2.10                     | 0.51              |
| 2:M:726:ILE:HG13 | 2:M:728:HIS:HB3  | 1.91                     | 0.51              |
| 2:M:73:LEU:HB3   | 2:M:94:LEU:HA    | 1.93                     | 0.51              |
| 3:N:1025:GLN:HA  | 3:N:1025:GLN:OE1 | 2.09                     | 0.51              |
| 3:N:1183:ILE:C   | 3:N:1184:GLN:HG3 | 2.29                     | 0.51              |
| 3:N:1402:ALA:HA  | 3:N:1415:VAL:CG2 | 2.40                     | 0.51              |
| 3:N:1380:GLU:O   | 3:N:1417:TRP:HB2 | 2.10                     | 0.51              |
| 3:N:249:TYR:CD2  | 3:N:288:MET:HE1  | 2.45                     | 0.51              |
| 3:N:470:LEU:O    | 3:N:471:GLU:C    | 2.48                     | 0.51              |
| 3:N:562:ALA:HB3  | 3:N:567:ILE:CD1  | 2.36                     | 0.51              |
| 3:N:807:ALA:H    | 3:N:809:PRO:HD2  | 1.73                     | 0.51              |
| 3:N:916:TYR:HH   | 3:N:1145:TYR:HH  | 1.56                     | 0.51              |
| 2:M:678:PRO:O    | 3:N:943:THR:HG23 | 2.10                     | 0.51              |
| 5:P:203:THR:HG22 | 5:P:204:GLY:N    | 2.25                     | 0.51              |
| 2:M:371:LYS:HA   | 5:P:280:GLN:OE1  | 2.09                     | 0.51              |
| 5:P:382:THR:HG22 | 5:P:397:ILE:HD12 | 1.91                     | 0.51              |
| 2:C:240:THR:O    | 2:C:242:LEU:N    | 2.44                     | 0.51              |
| 2:C:599:GLU:HB3  | 2:C:615:TYR:HD2  | 1.72                     | 0.51              |
| 2:C:724:ARG:HH21 | 2:C:734:LEU:HB3  | 1.74                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:773:LEU:CD1  | 2:C:777:ILE:HD11 | 2.40                     | 0.51              |
| 3:D:1006:ALA:O   | 3:D:1010:ASN:N   | 2.30                     | 0.51              |
| 3:D:1277:ILE:CG2 | 3:D:1278:ASP:H   | 2.11                     | 0.51              |
| 3:D:156:GLU:CD   | 3:D:156:GLU:H    | 2.12                     | 0.51              |
| 3:D:223:LEU:O    | 3:D:224:ARG:HD2  | 2.09                     | 0.51              |
| 3:D:241:ILE:CG2  | 3:D:242:LEU:N    | 2.73                     | 0.51              |
| 3:D:41:ARG:HE    | 3:D:48:ARG:NE    | 2.09                     | 0.51              |
| 3:D:629:SER:O    | 3:D:744:GLN:HG2  | 2.11                     | 0.51              |
| 3:D:709:HIS:O    | 3:D:712:GLY:N    | 2.40                     | 0.51              |
| 3:D:798:GLU:HG3  | 3:D:799:LYS:HB2  | 1.92                     | 0.51              |
| 3:D:907:GLU:O    | 3:D:908:LYS:C    | 2.48                     | 0.51              |
| 5:F:118:GLU:O    | 5:F:120:THR:N    | 2.44                     | 0.51              |
| 5:F:261:PRO:HB2  | 5:F:264:MET:CG   | 2.40                     | 0.51              |
| 1:K:1:MET:N      | 1:K:6:LEU:HD22   | 2.24                     | 0.51              |
| 2:M:928:LYS:O    | 2:M:931:GLY:N    | 2.44                     | 0.51              |
| 3:N:131:LYS:CB   | 3:N:456:MET:HE2  | 2.41                     | 0.51              |
| 3:N:186:VAL:O    | 3:N:189:GLN:HB2  | 2.10                     | 0.51              |
| 3:N:986:ARG:O    | 3:N:989:TYR:HB3  | 2.11                     | 0.51              |
| 5:P:126:LEU:O    | 5:P:129:GLU:HB3  | 2.09                     | 0.51              |
| 5:P:145:PRO:CG   | 5:P:150:THR:H    | 2.23                     | 0.51              |
| 5:P:244:ARG:O    | 5:P:248:ASN:ND2  | 2.44                     | 0.51              |
| 5:P:271:LEU:O    | 5:P:274:THR:N    | 2.41                     | 0.51              |
| 5:P:300:ASP:O    | 5:P:303:ARG:HB3  | 2.11                     | 0.51              |
| 5:P:376:ILE:HG22 | 5:P:377:ASP:N    | 2.26                     | 0.51              |
| 5:P:81:VAL:CG2   | 5:P:82:ARG:N     | 2.73                     | 0.51              |
| 1:B:57:TYR:O     | 1:B:140:MET:HB2  | 2.10                     | 0.51              |
| 1:B:144:VAL:HG12 | 1:B:145:ASP:N    | 2.25                     | 0.51              |
| 1:B:226:SER:O    | 1:B:228:PRO:HD3  | 2.10                     | 0.51              |
| 2:C:1005:MET:CE  | 3:D:648:MET:HB2  | 2.41                     | 0.51              |
| 2:C:145:GLY:HA3  | 2:C:276:LYS:CD   | 2.40                     | 0.51              |
| 2:C:195:LEU:HD12 | 2:C:238:LEU:CD2  | 2.41                     | 0.51              |
| 2:C:20:GLU:HA    | 2:C:23:VAL:HG22  | 1.91                     | 0.51              |
| 2:C:380:ALA:O    | 2:C:384:GLU:N    | 2.42                     | 0.51              |
| 2:C:512:ARG:HB3  | 2:C:523:ILE:HD11 | 1.93                     | 0.51              |
| 2:C:747:ALA:O    | 2:C:799:ILE:HA   | 2.10                     | 0.51              |
| 2:C:834:GLN:HB2  | 11:C:1128:HOH:O  | 2.10                     | 0.51              |
| 2:C:966:LEU:HD21 | 2:C:986:PRO:HG3  | 1.93                     | 0.51              |
| 3:D:1108:ARG:HE  | 3:D:1199:GLY:CA  | 2.22                     | 0.51              |
| 3:D:1237:THR:O   | 3:D:1255:GLY:HA3 | 2.10                     | 0.51              |
| 2:C:1046:ALA:CA  | 3:D:1472:ILE:HB  | 2.40                     | 0.51              |
| 3:D:33:ASN:O     | 3:D:37:LEU:CA    | 2.59                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:566:ILE:CG1   | 3:D:567:ILE:N     | 2.74                     | 0.51              |
| 3:D:674:ARG:HG3   | 3:D:674:ARG:HH11  | 1.76                     | 0.51              |
| 3:D:792:ILE:HG21  | 3:D:941:PHE:CE1   | 2.46                     | 0.51              |
| 3:D:880:ILE:O     | 3:D:883:ALA:HB3   | 2.10                     | 0.51              |
| 5:F:328:PHE:O     | 5:F:329:TYR:C     | 2.49                     | 0.51              |
| 5:F:358:LEU:HD21  | 5:F:370:LYS:NZ    | 2.25                     | 0.51              |
| 5:F:370:LYS:CG    | 5:F:371:LEU:N     | 2.73                     | 0.51              |
| 1:K:5:LYS:NZ      | 1:K:29:GLU:N      | 2.59                     | 0.51              |
| 1:L:91:ASN:ND2    | 1:L:93:SER:H      | 2.08                     | 0.51              |
| 2:M:343:GLN:O     | 2:M:346:VAL:HG22  | 2.10                     | 0.51              |
| 2:M:328:LEU:HG    | 2:M:433:THR:OG1   | 2.11                     | 0.51              |
| 2:M:41:ASN:O      | 2:M:46:ALA:N      | 2.43                     | 0.51              |
| 3:N:1403:LEU:HD23 | 3:N:1408:ILE:HD11 | 1.91                     | 0.51              |
| 3:N:128:TYR:CE1   | 3:N:461:ILE:HG13  | 2.45                     | 0.51              |
| 3:N:591:VAL:HG21  | 3:N:597:ASP:HA    | 1.92                     | 0.51              |
| 3:N:592:THR:HG23  | 3:N:600:LEU:CD2   | 2.36                     | 0.51              |
| 3:N:768:ASN:C     | 3:N:769:LEU:HD12  | 2.29                     | 0.51              |
| 3:N:767:HIS:HA    | 3:N:924:MET:CE    | 2.41                     | 0.51              |
| 3:N:95:LEU:CD1    | 3:N:99:ALA:HB2    | 2.41                     | 0.51              |
| 5:P:353:GLU:C     | 5:P:356:LYS:HB2   | 2.30                     | 0.51              |
| 5:P:361:LEU:CD1   | 5:P:362:SER:H     | 2.24                     | 0.51              |
| 1:A:104:GLU:HG2   | 1:A:105:GLY:N     | 2.25                     | 0.51              |
| 1:A:14:ARG:CB     | 1:B:233:VAL:HA    | 2.20                     | 0.51              |
| 2:C:129:ILE:HG12  | 2:C:134:ARG:HB2   | 1.91                     | 0.51              |
| 2:C:152:PRO:HG2   | 2:C:153:ALA:H     | 1.74                     | 0.51              |
| 2:C:185:LYS:CA    | 2:C:190:LYS:HB3   | 2.38                     | 0.51              |
| 2:C:205:GLU:N     | 2:C:209:ARG:NH1   | 2.58                     | 0.51              |
| 2:C:377:PRO:HG2   | 2:C:378:LEU:H     | 1.75                     | 0.51              |
| 2:C:881:ASN:N     | 2:C:881:ASN:ND2   | 2.45                     | 0.51              |
| 3:D:1269:LYS:CE   | 3:D:1269:LYS:H    | 2.23                     | 0.51              |
| 3:D:1367:HIS:O    | 3:D:1370:ILE:HB   | 2.10                     | 0.51              |
| 3:D:244:GLU:HA    | 3:D:309:GLY:C     | 2.31                     | 0.51              |
| 3:D:403:PHE:HB2   | 3:D:423:ASP:OD1   | 2.10                     | 0.51              |
| 3:D:136:ASP:N     | 3:D:453:ASP:O     | 2.41                     | 0.51              |
| 3:D:523:ASP:CA    | 3:D:526:PRO:HG3   | 2.39                     | 0.51              |
| 5:F:343:ASP:C     | 5:F:347:GLN:NE2   | 2.64                     | 0.51              |
| 1:K:101:LEU:C     | 1:K:102:LYS:HG3   | 2.30                     | 0.51              |
| 1:K:170:VAL:O     | 1:K:170:VAL:HG23  | 2.10                     | 0.51              |
| 1:K:38:ASN:HB3    | 1:K:39:PRO:CD     | 2.40                     | 0.51              |
| 2:M:183:SER:HB3   | 2:M:185:LYS:HE2   | 1.92                     | 0.51              |
| 2:M:677:MET:N     | 2:M:871:LEU:O     | 2.40                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:945:ARG:O    | 2:M:949:LYS:HG3   | 2.11                     | 0.51              |
| 3:N:421:LEU:HD11 | 3:N:429:SER:N     | 2.25                     | 0.51              |
| 3:N:653:PHE:HD1  | 3:N:653:PHE:N     | 2.07                     | 0.51              |
| 3:N:658:LEU:HA   | 3:N:661:MET:CE    | 2.34                     | 0.51              |
| 3:N:960:LYS:HG2  | 3:N:964:LEU:HD11  | 1.92                     | 0.51              |
| 5:P:355:GLU:HA   | 5:P:358:LEU:HD23  | 1.92                     | 0.51              |
| 5:P:386:VAL:CG2  | 5:P:387:GLY:H     | 2.22                     | 0.51              |
| 1:B:175:ARG:NH1  | 1:B:175:ARG:HG2   | 2.26                     | 0.51              |
| 2:C:1102:LEU:O   | 3:D:7:LYS:O       | 2.29                     | 0.51              |
| 2:C:266:ARG:HD2  | 2:C:273:GLY:CA    | 2.40                     | 0.51              |
| 2:C:346:VAL:CG2  | 2:C:347:GLY:H     | 2.19                     | 0.51              |
| 2:C:774:LEU:HD13 | 2:C:775:ARG:N     | 2.26                     | 0.51              |
| 3:D:957:PRO:CG   | 3:D:1010:ASN:HD22 | 2.07                     | 0.51              |
| 3:D:1126:ASP:HA  | 3:D:1128:VAL:O    | 2.10                     | 0.51              |
| 3:D:135:LEU:CD2  | 3:D:135:LEU:H     | 2.16                     | 0.51              |
| 3:D:671:LYS:O    | 3:D:674:ARG:HB2   | 2.11                     | 0.51              |
| 3:D:85:VAL:CG2   | 3:D:89:ARG:NE     | 2.73                     | 0.51              |
| 3:D:969:ARG:O    | 3:D:972:LEU:HB2   | 2.11                     | 0.51              |
| 2:M:260:LEU:CD1  | 2:M:288:ARG:HG2   | 2.41                     | 0.51              |
| 2:M:599:GLU:HA   | 2:M:599:GLU:OE1   | 2.10                     | 0.51              |
| 2:M:626:ARG:HH11 | 2:M:626:ARG:HG3   | 1.76                     | 0.51              |
| 2:M:745:ILE:CG2  | 2:M:746:GLY:N     | 2.73                     | 0.51              |
| 3:N:1035:ILE:O   | 3:N:1036:ARG:C    | 2.49                     | 0.51              |
| 3:N:1150:ALA:O   | 3:N:1151:ARG:HD3  | 2.10                     | 0.51              |
| 3:N:1445:HIS:O   | 3:N:1449:GLU:OE2  | 2.27                     | 0.51              |
| 3:N:1464:GLU:CG  | 3:N:1465:ASN:N    | 2.74                     | 0.51              |
| 3:N:173:PRO:HA   | 3:N:209:ARG:HH11  | 1.76                     | 0.51              |
| 3:N:228:ALA:HA   | 3:N:326:GLU:OE1   | 2.11                     | 0.51              |
| 3:N:411:THR:HA   | 3:N:435:VAL:HG12  | 1.91                     | 0.51              |
| 3:N:686:GLU:H    | 3:N:686:GLU:CD    | 2.14                     | 0.51              |
| 3:N:807:ALA:HB2  | 3:N:833:GLU:OE1   | 2.10                     | 0.51              |
| 3:N:828:LYS:CD   | 3:N:828:LYS:H     | 2.23                     | 0.51              |
| 3:N:83:SER:O     | 3:N:86:ARG:HB2    | 2.11                     | 0.51              |
| 3:N:87:ARG:CB    | 3:N:523:ASP:HB2   | 2.41                     | 0.51              |
| 3:N:89:ARG:O     | 3:N:521:PRO:HG3   | 2.11                     | 0.51              |
| 3:N:936:TYR:C    | 3:N:936:TYR:CD2   | 2.84                     | 0.51              |
| 3:N:961:LYS:O    | 3:N:964:LEU:HB2   | 2.11                     | 0.51              |
| 5:P:262:VAL:C    | 5:P:264:MET:H     | 2.13                     | 0.51              |
| 5:P:382:THR:HG22 | 5:P:394:ARG:CB    | 2.40                     | 0.51              |
| 5:P:393:THR:HG22 | 5:P:394:ARG:N     | 2.26                     | 0.51              |
| 1:B:175:ARG:HH11 | 1:B:175:ARG:HG2   | 1.74                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:43:ILE:HA     | 1:B:46:SER:OG    | 2.11                     | 0.51              |
| 1:B:43:ILE:HG23   | 1:B:47:SER:HB2   | 1.93                     | 0.51              |
| 2:C:142:ARG:HD3   | 2:C:163:ILE:CD1  | 2.41                     | 0.51              |
| 2:C:184:MET:CG    | 2:C:193:LEU:HD13 | 2.40                     | 0.51              |
| 2:C:444:PRO:HD2   | 2:C:452:ILE:O    | 2.09                     | 0.51              |
| 2:C:628:PHE:CD1   | 2:C:628:PHE:N    | 2.77                     | 0.51              |
| 2:C:946:ARG:HE    | 3:D:796:ARG:NH2  | 2.09                     | 0.51              |
| 2:C:987:ILE:HD13  | 3:D:948:THR:HG23 | 1.92                     | 0.51              |
| 2:C:888:THR:HA    | 2:C:991:GLN:O    | 2.11                     | 0.51              |
| 3:D:1015:TYR:N    | 3:D:1016:PRO:CD  | 2.74                     | 0.51              |
| 3:D:1040:GLY:O    | 3:D:1060:SER:HB3 | 2.10                     | 0.51              |
| 3:D:1296:SER:HB3  | 3:D:1299:PHE:CD1 | 2.46                     | 0.51              |
| 3:D:1374:GLN:HA   | 3:D:1377:LYS:HB2 | 1.92                     | 0.51              |
| 3:D:1451:ALA:O    | 3:D:1454:GLY:N   | 2.41                     | 0.51              |
| 3:D:703:ASN:HB3   | 3:D:746:ALA:HB3  | 1.93                     | 0.51              |
| 3:D:756:GLN:O     | 3:D:759:ALA:HB3  | 2.11                     | 0.51              |
| 3:D:769:LEU:N     | 3:D:769:LEU:CD1  | 2.73                     | 0.51              |
| 2:M:1015:LEU:O    | 2:M:1018:GLN:NE2 | 2.44                     | 0.51              |
| 2:M:643:VAL:HG23  | 2:M:647:GLN:NE2  | 2.26                     | 0.51              |
| 3:N:1492:LEU:HD11 | 4:O:74:VAL:HG21  | 1.93                     | 0.51              |
| 3:N:22:SER:HB2    | 3:N:24:GLY:O     | 2.10                     | 0.51              |
| 3:N:274:ARG:CB    | 3:N:279:VAL:HG21 | 2.31                     | 0.51              |
| 3:N:399:ARG:O     | 3:N:401:TYR:HD1  | 1.94                     | 0.51              |
| 3:N:555:LYS:CA    | 3:N:558:LEU:HD12 | 2.37                     | 0.51              |
| 3:N:760:ARG:O     | 3:N:764:LEU:HB2  | 2.11                     | 0.51              |
| 3:N:826:PRO:HB3   | 3:N:828:LYS:NZ   | 2.26                     | 0.51              |
| 4:O:29:GLN:C      | 4:O:31:LEU:H     | 2.13                     | 0.51              |
| 4:O:40:LEU:CG     | 4:O:44:GLU:HB2   | 2.40                     | 0.51              |
| 5:P:156:VAL:HG23  | 5:P:157:GLU:CD   | 2.30                     | 0.51              |
| 5:P:236:SER:O     | 5:P:238:TYR:N    | 2.44                     | 0.51              |
| 5:P:306:GLU:OE1   | 5:P:306:GLU:HA   | 2.11                     | 0.51              |
| 5:P:330:GLY:CA    | 5:P:333:ILE:HD13 | 2.40                     | 0.51              |
| 5:P:368:VAL:CG2   | 5:P:369:LEU:H    | 1.95                     | 0.51              |
| 5:P:401:GLU:HG2   | 5:P:402:ASN:N    | 2.25                     | 0.51              |
| 5:P:92:PRO:C      | 5:P:94:LEU:H     | 2.13                     | 0.51              |
| 1:B:58:ILE:HG23   | 1:B:61:VAL:HB    | 1.88                     | 0.51              |
| 1:B:87:VAL:HG12   | 1:B:122:ILE:HA   | 1.91                     | 0.51              |
| 2:C:129:ILE:HG12  | 2:C:134:ARG:CB   | 2.41                     | 0.51              |
| 2:C:200:LEU:HB3   | 2:C:202:TYR:CE2  | 2.46                     | 0.51              |
| 2:C:695:LEU:HD22  | 2:C:832:LYS:HG2  | 1.93                     | 0.51              |
| 3:D:1288:GLU:N    | 3:D:1288:GLU:OE1 | 2.44                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1336:LEU:O    | 3:D:1340:GLY:N    | 2.43                     | 0.51              |
| 3:D:23:TYR:CD2    | 3:D:89:ARG:HD3    | 2.46                     | 0.51              |
| 3:D:367:ILE:HB    | 3:D:377:VAL:HG11  | 1.87                     | 0.51              |
| 3:D:441:ARG:HD3   | 3:D:443:VAL:CG2   | 2.40                     | 0.51              |
| 3:D:617:ASN:HB3   | 3:D:619:LEU:HG    | 1.92                     | 0.51              |
| 3:D:701:LEU:HD21  | 3:D:715:ALA:HB2   | 1.92                     | 0.51              |
| 3:D:59:ALA:HB3    | 3:D:76:CYS:HB2    | 1.93                     | 0.51              |
| 3:D:936:TYR:CD2   | 3:D:936:TYR:C     | 2.84                     | 0.51              |
| 5:F:213:ILE:HG22  | 5:F:217:ASN:ND2   | 2.25                     | 0.51              |
| 5:F:231:ARG:CB    | 5:F:233:PHE:CE2   | 2.94                     | 0.51              |
| 5:F:408:LEU:HG    | 5:F:409:LYS:N     | 2.26                     | 0.51              |
| 1:K:40:LEU:O      | 1:K:41:ARG:C      | 2.48                     | 0.51              |
| 2:M:1099:VAL:HA   | 3:N:9:ARG:O       | 2.10                     | 0.51              |
| 2:M:186:VAL:CG1   | 2:M:187:ASN:H     | 2.10                     | 0.51              |
| 2:M:205:GLU:HA    | 2:M:209:ARG:HD3   | 1.92                     | 0.51              |
| 2:M:578:VAL:HG13  | 2:M:671:ASN:CG    | 2.32                     | 0.51              |
| 2:M:725:ASP:OD2   | 2:M:783:ARG:NH1   | 2.41                     | 0.51              |
| 2:M:768:THR:HG22  | 2:M:770:GLU:H     | 1.75                     | 0.51              |
| 3:N:1125:PRO:HA   | 3:N:1131:SER:O    | 2.10                     | 0.51              |
| 3:N:1254:GLN:HG2  | 3:N:1255:GLY:H    | 1.75                     | 0.51              |
| 3:N:1282:ARG:HB3  | 3:N:1293:PHE:HB3  | 1.92                     | 0.51              |
| 3:N:470:LEU:HB2   | 3:N:503:LEU:CG    | 2.41                     | 0.51              |
| 3:N:584:ASN:OD1   | 3:N:585:GLY:N     | 2.44                     | 0.51              |
| 2:M:987:ILE:HD12  | 3:N:948:THR:CG2   | 2.41                     | 0.51              |
| 3:N:1485:GLN:N    | 4:O:76:GLY:O      | 2.35                     | 0.51              |
| 5:P:172:ARG:O     | 5:P:176:ILE:HG13  | 2.11                     | 0.51              |
| 5:P:207:LEU:O     | 5:P:212:LEU:HD21  | 2.11                     | 0.51              |
| 5:P:256:ARG:HH21  | 5:P:311:ALA:HA    | 1.75                     | 0.51              |
| 5:P:359:SER:C     | 5:P:361:LEU:H     | 2.14                     | 0.51              |
| 1:A:178:ALA:HB2   | 2:C:864:GLY:CA    | 2.39                     | 0.51              |
| 2:C:395:LYS:HD3   | 2:C:397:GLU:OE1   | 2.11                     | 0.51              |
| 2:C:906:PHE:CE2   | 3:D:1067:VAL:HA   | 2.46                     | 0.51              |
| 2:C:910:LYS:C     | 2:C:914:ILE:HD13  | 2.31                     | 0.51              |
| 3:D:1011:PHE:HE1  | 3:D:1018:ASN:ND2  | 2.09                     | 0.51              |
| 3:D:1067:VAL:HG13 | 3:D:1068:LEU:H    | 1.74                     | 0.51              |
| 3:D:1106:VAL:CG1  | 3:D:1107:VAL:N    | 2.74                     | 0.51              |
| 3:D:1367:HIS:O    | 3:D:1371:VAL:HG23 | 2.11                     | 0.51              |
| 3:D:295:GLY:O     | 3:D:296:GLU:HG3   | 2.10                     | 0.51              |
| 3:D:425:GLY:C     | 3:D:427:VAL:H     | 2.14                     | 0.51              |
| 2:C:987:ILE:HG23  | 3:D:948:THR:HG21  | 1.91                     | 0.51              |
| 3:D:999:THR:O     | 3:D:1003:VAL:HG23 | 2.11                     | 0.51              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:E:20:THR:O     | 4:E:21:VAL:C     | 2.49                     | 0.51              |
| 4:E:87:LYS:HE3   | 4:E:91:ARG:HH22  | 1.76                     | 0.51              |
| 5:F:269:ASN:O    | 5:F:270:LYS:C    | 2.49                     | 0.51              |
| 1:K:219:ARG:HH11 | 1:K:219:ARG:HG2  | 1.74                     | 0.51              |
| 1:L:12:THR:OG1   | 1:L:24:VAL:HB    | 2.11                     | 0.51              |
| 1:L:57:TYR:O     | 1:L:140:MET:HB2  | 2.11                     | 0.51              |
| 2:M:12:VAL:HG23  | 2:M:13:ILE:N     | 2.26                     | 0.51              |
| 2:M:18:LEU:C     | 2:M:20:GLU:H     | 2.15                     | 0.51              |
| 2:M:243:ARG:CG   | 2:M:244:PRO:CA   | 2.88                     | 0.51              |
| 2:M:343:GLN:HG2  | 2:M:385:PHE:CB   | 2.41                     | 0.51              |
| 2:M:675:ALA:O    | 2:M:677:MET:HG2  | 2.10                     | 0.51              |
| 3:N:1083:ASP:O   | 3:N:1086:LEU:HB2 | 2.10                     | 0.51              |
| 3:N:1406:ARG:HG2 | 3:N:1412:LYS:CD  | 2.41                     | 0.51              |
| 3:N:1495:ILE:CG2 | 3:N:1496:GLU:N   | 2.71                     | 0.51              |
| 3:N:191:LEU:HB3  | 3:N:195:VAL:O    | 2.10                     | 0.51              |
| 3:N:406:ASP:N    | 3:N:423:ASP:OD1  | 2.44                     | 0.51              |
| 3:N:411:THR:HG21 | 5:P:179:GLU:HG2  | 1.92                     | 0.51              |
| 3:N:490:ALA:O    | 3:N:493:ARG:HG2  | 2.11                     | 0.51              |
| 3:N:561:GLY:HA2  | 5:P:140:ARG:HH21 | 1.75                     | 0.51              |
| 1:L:176:ARG:HD3  | 3:N:884:ARG:NH2  | 2.26                     | 0.51              |
| 3:N:971:LEU:O    | 3:N:974:ILE:HB   | 2.11                     | 0.51              |
| 4:O:40:LEU:HG    | 4:O:44:GLU:HB2   | 1.93                     | 0.51              |
| 1:A:34:VAL:C     | 1:A:36:LEU:H     | 2.14                     | 0.51              |
| 2:C:157:ARG:NH1  | 2:C:158:TYR:OH   | 2.44                     | 0.51              |
| 2:C:151:ASP:N    | 2:C:158:TYR:HA   | 2.18                     | 0.51              |
| 2:C:144:PRO:CB   | 2:C:266:ARG:HB3  | 2.40                     | 0.51              |
| 2:C:628:PHE:HD1  | 2:C:628:PHE:N    | 2.09                     | 0.51              |
| 2:C:687:ALA:HB1  | 2:C:850:ALA:HB2  | 1.92                     | 0.51              |
| 3:D:1286:THR:CB  | 3:D:1289:LYS:H   | 2.23                     | 0.51              |
| 3:D:14:SER:O     | 3:D:18:ILE:N     | 2.30                     | 0.51              |
| 3:D:27:GLU:C     | 3:D:28:LYS:HD3   | 2.30                     | 0.51              |
| 3:D:322:VAL:HG22 | 3:D:333:LEU:HD22 | 1.93                     | 0.51              |
| 3:D:444:VAL:HG23 | 3:D:444:VAL:O    | 2.11                     | 0.51              |
| 5:F:235:PHE:O    | 5:F:238:TYR:HB3  | 2.11                     | 0.51              |
| 1:L:56:VAL:HG12  | 1:L:57:TYR:H     | 1.76                     | 0.51              |
| 1:L:89:PHE:HD2   | 1:L:94:LEU:HB2   | 1.75                     | 0.51              |
| 2:M:203:ASP:OD1  | 2:M:205:GLU:HB3  | 2.11                     | 0.51              |
| 2:M:470:PRO:HG3  | 2:M:485:TYR:OH   | 2.09                     | 0.51              |
| 2:M:73:LEU:CB    | 2:M:93:PRO:O     | 2.59                     | 0.51              |
| 2:M:73:LEU:O     | 2:M:73:LEU:HD12  | 2.11                     | 0.51              |
| 3:N:1422:MET:SD  | 3:N:1427:SER:HA  | 2.51                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1472:ILE:HD13 | 3:N:1473:PRO:CD  | 2.41                     | 0.51              |
| 3:N:521:PRO:C     | 3:N:525:ARG:HH12 | 2.14                     | 0.51              |
| 3:N:562:ALA:CB    | 3:N:567:ILE:HD11 | 2.37                     | 0.51              |
| 3:N:582:LEU:HA    | 3:N:603:LEU:HD12 | 1.92                     | 0.51              |
| 3:N:648:MET:O     | 3:N:649:ALA:C    | 2.50                     | 0.51              |
| 3:N:911:LEU:O     | 3:N:912:LYS:C    | 2.49                     | 0.51              |
| 3:N:961:LYS:HA    | 3:N:964:LEU:HD12 | 1.93                     | 0.51              |
| 3:N:995:LEU:HG    | 3:N:996:TRP:N    | 2.25                     | 0.51              |
| 4:O:30:LEU:O      | 4:O:34:GLY:O     | 2.29                     | 0.51              |
| 5:P:111:GLU:HA    | 5:P:114:LYS:CG   | 2.41                     | 0.51              |
| 5:P:150:THR:O     | 5:P:152:ASP:N    | 2.44                     | 0.51              |
| 5:P:291:ILE:O     | 5:P:292:ALA:C    | 2.49                     | 0.51              |
| 5:P:380:GLU:HA    | 5:P:385:GLU:CD   | 2.31                     | 0.51              |
| 1:B:112:ARG:HH22  | 1:B:125:PRO:HB2  | 1.76                     | 0.50              |
| 1:B:112:ARG:NH2   | 1:B:125:PRO:HB2  | 2.25                     | 0.50              |
| 2:C:1012:PRO:HB2  | 2:C:1021:LEU:O   | 2.11                     | 0.50              |
| 2:C:115:LEU:N     | 2:C:115:LEU:HD23 | 2.25                     | 0.50              |
| 2:C:45:GLN:HA     | 2:C:48:PHE:HD1   | 1.76                     | 0.50              |
| 3:D:349:PRO:CB    | 5:F:97:GLU:HG2   | 2.41                     | 0.50              |
| 3:D:583:ASP:HA    | 3:D:602:SER:OG   | 2.11                     | 0.50              |
| 3:D:653:PHE:O     | 3:D:654:LYS:C    | 2.48                     | 0.50              |
| 5:F:138:SER:HA    | 5:F:141:VAL:HG13 | 1.93                     | 0.50              |
| 5:F:251:ILE:O     | 5:F:255:ALA:CB   | 2.59                     | 0.50              |
| 5:F:350:LEU:O     | 5:F:352:GLU:N    | 2.44                     | 0.50              |
| 1:K:56:VAL:HG21   | 1:K:82:LEU:HD12  | 1.93                     | 0.50              |
| 1:L:88:ARG:O      | 1:L:120:VAL:HA   | 2.10                     | 0.50              |
| 1:L:19:GLU:HA     | 1:L:201:THR:OG1  | 2.10                     | 0.50              |
| 1:K:9:PRO:HD2     | 1:L:224:TYR:CD1  | 2.45                     | 0.50              |
| 2:M:1036:GLU:O    | 2:M:1037:VAL:C   | 2.50                     | 0.50              |
| 2:M:211:LEU:O     | 2:M:213:ALA:N    | 2.44                     | 0.50              |
| 3:N:1344:VAL:HG13 | 3:N:1345:GLU:N   | 2.26                     | 0.50              |
| 3:N:319:ALA:HA    | 3:N:336:PHE:O    | 2.10                     | 0.50              |
| 3:N:402:PRO:CB    | 3:N:443:VAL:HG22 | 2.41                     | 0.50              |
| 3:N:598:ARG:HG2   | 3:N:598:ARG:NH1  | 2.27                     | 0.50              |
| 3:N:605:ASP:N     | 3:N:605:ASP:OD1  | 2.34                     | 0.50              |
| 3:N:610:LYS:NZ    | 3:N:1441:GLN:HA  | 2.26                     | 0.50              |
| 3:N:618:LEU:N     | 3:N:618:LEU:HD23 | 2.25                     | 0.50              |
| 1:B:151:VAL:O     | 1:B:168:ASP:HA   | 2.11                     | 0.50              |
| 1:B:186:LEU:C     | 1:B:188:GLN:H    | 2.15                     | 0.50              |
| 2:C:151:ASP:HB2   | 2:C:158:TYR:HA   | 1.93                     | 0.50              |
| 2:C:249:LYS:O     | 2:C:251:ASP:N    | 2.44                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:266:ARG:HD2   | 2:C:273:GLY:HA3  | 1.93                     | 0.50              |
| 2:C:569:VAL:HG12  | 2:C:996:LYS:O    | 2.12                     | 0.50              |
| 2:C:759:THR:HG22  | 2:C:787:ASP:HA   | 1.93                     | 0.50              |
| 2:C:773:LEU:HD11  | 2:C:777:ILE:HD11 | 1.92                     | 0.50              |
| 2:C:874:LEU:HB3   | 3:D:1029:ARG:CD  | 2.41                     | 0.50              |
| 2:C:94:LEU:N      | 2:C:116:GLY:O    | 2.43                     | 0.50              |
| 3:D:1466:VAL:C    | 3:D:1468:LEU:N   | 2.65                     | 0.50              |
| 3:D:1478:SER:O    | 3:D:1482:ARG:HG3 | 2.11                     | 0.50              |
| 3:D:510:GLU:O     | 3:D:513:ILE:HG22 | 2.12                     | 0.50              |
| 5:F:116:LEU:O     | 5:F:117:SER:C    | 2.50                     | 0.50              |
| 5:F:132:ARG:O     | 5:F:133:ALA:C    | 2.49                     | 0.50              |
| 5:F:358:LEU:CD2   | 5:F:370:LYS:HZ2  | 2.23                     | 0.50              |
| 5:F:382:THR:HG23  | 5:F:397:ILE:HG21 | 1.92                     | 0.50              |
| 1:K:220:GLU:O     | 1:K:223:THR:HB   | 2.11                     | 0.50              |
| 1:L:13:VAL:HG22   | 1:L:14:ARG:N     | 2.26                     | 0.50              |
| 1:L:83:LYS:NZ     | 1:L:168:ASP:HB2  | 2.26                     | 0.50              |
| 2:M:355:VAL:C     | 2:M:358:ARG:HG3  | 2.32                     | 0.50              |
| 2:M:550:LEU:HD23  | 2:M:905:ILE:HD11 | 1.92                     | 0.50              |
| 2:M:897:LEU:HD21  | 2:M:920:GLN:HB3  | 1.92                     | 0.50              |
| 2:M:943:VAL:O     | 2:M:944:LEU:C    | 2.49                     | 0.50              |
| 2:M:998:TYR:CE2   | 2:M:1000:MET:HA  | 2.47                     | 0.50              |
| 3:N:1341:PRO:O    | 3:N:1345:GLU:HG3 | 2.11                     | 0.50              |
| 3:N:1404:ASN:HB3  | 3:N:1409:ALA:HB3 | 1.92                     | 0.50              |
| 3:N:1465:ASN:HD22 | 3:N:1472:ILE:HA  | 1.76                     | 0.50              |
| 3:N:283:PHE:O     | 3:N:284:LEU:HD23 | 2.11                     | 0.50              |
| 3:N:437:VAL:HG12  | 3:N:438:ASP:O    | 2.10                     | 0.50              |
| 3:N:560:GLN:HG3   | 5:P:184:ARG:NH2  | 2.27                     | 0.50              |
| 3:N:820:GLU:HA    | 3:N:825:ALA:H    | 1.76                     | 0.50              |
| 1:A:23:PHE:N      | 1:A:23:PHE:CD1   | 2.79                     | 0.50              |
| 1:A:41:ARG:HG2    | 1:A:45:LEU:HD11  | 1.93                     | 0.50              |
| 2:C:1008:ARG:NH2  | 2:C:1012:PRO:O   | 2.44                     | 0.50              |
| 2:C:233:GLU:HB2   | 2:C:237:ARG:CZ   | 2.41                     | 0.50              |
| 2:C:3:ILE:CD1     | 2:C:5:ARG:HE     | 2.25                     | 0.50              |
| 3:D:1103:HIS:CG   | 3:D:1104:GLU:N   | 2.79                     | 0.50              |
| 3:D:1286:THR:C    | 3:D:1288:GLU:H   | 2.13                     | 0.50              |
| 3:D:1291:SER:HA   | 3:D:1305:LEU:CD2 | 2.41                     | 0.50              |
| 3:D:1342:GLU:H    | 3:D:1342:GLU:CD  | 2.14                     | 0.50              |
| 3:D:1101:VAL:HA   | 3:D:1428:ALA:HB2 | 1.92                     | 0.50              |
| 3:D:256:GLU:HA    | 3:D:272:LEU:HD13 | 1.92                     | 0.50              |
| 3:D:355:VAL:HG13  | 3:D:359:ALA:HB3  | 1.92                     | 0.50              |
| 2:C:1031:ARG:CB   | 3:D:622:ARG:HH12 | 2.25                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:70:GLY:HA2   | 3:D:80:VAL:HG23  | 1.92                     | 0.50              |
| 2:M:1110:ASP:OD1 | 2:M:1113:GLU:N   | 2.44                     | 0.50              |
| 2:M:261:ILE:HG22 | 2:M:262:ALA:H    | 1.75                     | 0.50              |
| 2:M:483:VAL:HG22 | 2:M:484:VAL:N    | 2.26                     | 0.50              |
| 2:M:486:MET:HG3  | 2:M:490:GLU:HB2  | 1.91                     | 0.50              |
| 2:M:605:LYS:O    | 2:M:606:VAL:HG13 | 2.11                     | 0.50              |
| 2:M:606:VAL:CG1  | 2:M:611:ILE:HG23 | 2.39                     | 0.50              |
| 2:M:398:THR:N    | 2:M:633:GLN:HG3  | 2.27                     | 0.50              |
| 2:M:726:ILE:C    | 2:M:728:HIS:N    | 2.65                     | 0.50              |
| 3:N:1196:THR:HB  | 3:N:1199:GLY:C   | 2.32                     | 0.50              |
| 3:N:1404:ASN:OD1 | 3:N:1409:ALA:HB2 | 2.11                     | 0.50              |
| 3:N:1409:ALA:C   | 3:N:1411:GLY:N   | 2.64                     | 0.50              |
| 3:N:141:ILE:CD1  | 3:N:450:TYR:H    | 2.23                     | 0.50              |
| 3:N:1476:THR:HB  | 4:O:21:VAL:CG2   | 2.40                     | 0.50              |
| 3:N:1483:PHE:N   | 3:N:1483:PHE:CD1 | 2.78                     | 0.50              |
| 3:N:261:LEU:HD21 | 3:N:290:PRO:HB2  | 1.94                     | 0.50              |
| 3:N:298:VAL:O    | 3:N:298:VAL:HG12 | 2.11                     | 0.50              |
| 3:N:432:TYR:N    | 3:N:432:TYR:CD1  | 2.79                     | 0.50              |
| 3:N:462:GLN:O    | 3:N:466:LYS:HG3  | 2.11                     | 0.50              |
| 3:N:928:ALA:O    | 3:N:929:ARG:C    | 2.50                     | 0.50              |
| 5:P:101:GLU:HA   | 5:P:104:ARG:HH12 | 1.72                     | 0.50              |
| 5:P:119:ILE:HG22 | 5:P:119:ILE:O    | 2.10                     | 0.50              |
| 5:P:282:LEU:O    | 5:P:284:ARG:N    | 2.41                     | 0.50              |
| 5:P:412:GLU:C    | 5:P:414:ARG:N    | 2.63                     | 0.50              |
| 1:A:18:ARG:NE    | 1:A:88:ARG:NH2   | 2.59                     | 0.50              |
| 2:C:23:VAL:CA    | 2:C:121:MET:HE1  | 2.37                     | 0.50              |
| 2:C:838:LYS:HE3  | 2:C:997:LEU:CB   | 2.41                     | 0.50              |
| 3:D:1103:HIS:HA  | 3:D:1223:ILE:CD1 | 2.41                     | 0.50              |
| 3:D:113:GLY:HA3  | 3:D:124:GLU:CD   | 2.31                     | 0.50              |
| 3:D:1269:LYS:CD  | 3:D:1269:LYS:H   | 2.25                     | 0.50              |
| 3:D:1294:VAL:C   | 3:D:1295:GLU:HG3 | 2.32                     | 0.50              |
| 3:D:1341:PRO:O   | 3:D:1344:VAL:N   | 2.44                     | 0.50              |
| 3:D:1424:VAL:CG2 | 3:D:1425:THR:N   | 2.75                     | 0.50              |
| 3:D:225:LEU:CD1  | 3:D:242:LEU:HD11 | 2.37                     | 0.50              |
| 3:D:33:ASN:O     | 3:D:37:LEU:HA    | 2.12                     | 0.50              |
| 3:D:807:ALA:N    | 3:D:809:PRO:HD2  | 2.26                     | 0.50              |
| 3:D:993:LEU:O    | 3:D:994:GLN:C    | 2.50                     | 0.50              |
| 4:E:75:PHE:C     | 4:E:79:LEU:HD11  | 2.31                     | 0.50              |
| 5:F:343:ASP:O    | 5:F:344:ALA:C    | 2.50                     | 0.50              |
| 5:F:397:ILE:O    | 5:F:398:ARG:C    | 2.49                     | 0.50              |
| 5:F:81:VAL:HG23  | 5:F:82:ARG:HG3   | 1.93                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:100:LEU:HB3   | 1:L:115:LEU:HD22 | 1.92                     | 0.50              |
| 1:L:151:VAL:HG21  | 1:L:171:PHE:HE1  | 1.76                     | 0.50              |
| 2:M:100:LEU:HD23  | 2:M:368:THR:CG2  | 2.39                     | 0.50              |
| 2:M:1055:LEU:CD1  | 2:M:1079:PRO:HG3 | 2.40                     | 0.50              |
| 2:M:157:ARG:HG3   | 2:M:158:TYR:H    | 1.75                     | 0.50              |
| 2:M:224:GLU:CB    | 2:M:227:PHE:HB2  | 2.42                     | 0.50              |
| 2:M:470:PRO:HG3   | 2:M:485:TYR:CE2  | 2.45                     | 0.50              |
| 2:M:654:LEU:HD12  | 2:M:655:LEU:N    | 2.22                     | 0.50              |
| 2:M:685:GLU:O     | 2:M:686:ASP:HB2  | 2.10                     | 0.50              |
| 2:M:728:HIS:NE2   | 2:M:730:SER:HB3  | 2.26                     | 0.50              |
| 2:M:781:LYS:CA    | 2:M:781:LYS:HE2  | 2.35                     | 0.50              |
| 2:M:890:LEU:O     | 2:M:893:ALA:HB3  | 2.12                     | 0.50              |
| 3:N:1099:VAL:O    | 3:N:1103:HIS:HB3 | 2.12                     | 0.50              |
| 3:N:264:LEU:HB2   | 3:N:267:GLY:CA   | 2.41                     | 0.50              |
| 3:N:455:ARG:CB    | 3:N:460:ALA:HB2  | 2.41                     | 0.50              |
| 3:N:536:ALA:HA    | 5:P:315:VAL:O    | 2.11                     | 0.50              |
| 3:N:656:PHE:HD1   | 3:N:656:PHE:H    | 1.56                     | 0.50              |
| 3:N:655:PRO:O     | 3:N:658:LEU:HB2  | 2.11                     | 0.50              |
| 3:N:812:ALA:HA    | 3:N:816:HIS:H    | 1.77                     | 0.50              |
| 3:N:986:ARG:HD3   | 3:N:989:TYR:HD2  | 1.76                     | 0.50              |
| 1:A:56:VAL:HG13   | 1:A:141:GLU:O    | 2.10                     | 0.50              |
| 2:C:328:LEU:HD11  | 2:C:434:HIS:HA   | 1.93                     | 0.50              |
| 2:C:437:ARG:HA    | 2:C:459:ALA:HB2  | 1.94                     | 0.50              |
| 2:C:882:LEU:HD12  | 3:D:1061:PHE:HB3 | 1.94                     | 0.50              |
| 2:C:928:LYS:O     | 2:C:931:GLY:N    | 2.43                     | 0.50              |
| 3:D:1335:LEU:HD21 | 3:D:1344:VAL:HA  | 1.93                     | 0.50              |
| 3:D:356:PRO:O     | 3:D:385:VAL:HG11 | 2.12                     | 0.50              |
| 2:C:1052:MET:SD   | 3:D:623:VAL:HG21 | 2.52                     | 0.50              |
| 3:D:968:ASP:O     | 3:D:971:LEU:HB2  | 2.12                     | 0.50              |
| 4:E:40:LEU:HD21   | 4:E:44:GLU:HB2   | 1.94                     | 0.50              |
| 3:D:925:GLU:OE2   | 4:E:6:ILE:HG22   | 2.11                     | 0.50              |
| 5:F:403:LYS:O     | 5:F:407:LYS:HB2  | 2.10                     | 0.50              |
| 1:K:100:LEU:HD13  | 1:K:115:LEU:HD12 | 1.93                     | 0.50              |
| 1:K:53:VAL:HG21   | 1:K:82:LEU:HB3   | 1.94                     | 0.50              |
| 1:L:112:ARG:HH21  | 1:L:126:ASP:CG   | 2.14                     | 0.50              |
| 2:M:1007:ALA:HB1  | 3:N:648:MET:HG3  | 1.92                     | 0.50              |
| 2:M:95:TYR:CE2    | 2:M:114:PHE:HB3  | 2.46                     | 0.50              |
| 2:M:138:SER:O     | 2:M:410:ILE:HA   | 2.12                     | 0.50              |
| 2:M:567:GLN:HB2   | 2:M:997:LEU:HD22 | 1.93                     | 0.50              |
| 3:N:1305:LEU:N    | 3:N:1305:LEU:CD2 | 2.74                     | 0.50              |
| 3:N:1394:VAL:O    | 3:N:1398:TRP:NE1 | 2.44                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:217:LYS:CD   | 3:N:262:LYS:NZ    | 2.74                     | 0.50              |
| 3:N:269:PHE:HD1  | 3:N:283:PHE:HB2   | 1.77                     | 0.50              |
| 3:N:676:MET:O    | 3:N:676:MET:SD    | 2.70                     | 0.50              |
| 3:N:785:ILE:HG12 | 3:N:939:PHE:HE2   | 1.75                     | 0.50              |
| 3:N:965:GLU:C    | 3:N:965:GLU:CD    | 2.70                     | 0.50              |
| 3:N:995:LEU:O    | 3:N:998:GLU:HB3   | 2.11                     | 0.50              |
| 5:P:155:THR:O    | 5:P:159:ILE:HG12  | 2.11                     | 0.50              |
| 5:P:273:ARG:O    | 5:P:277:GLN:HG3   | 2.12                     | 0.50              |
| 2:M:817:PRO:HB3  | 5:P:309:LYS:HE2   | 1.93                     | 0.50              |
| 1:A:49:PRO:HA    | 1:A:147:GLY:O     | 2.12                     | 0.50              |
| 1:B:38:ASN:O     | 1:B:41:ARG:HB3    | 2.12                     | 0.50              |
| 2:C:384:GLU:OE2  | 2:C:388:ARG:NH2   | 2.42                     | 0.50              |
| 2:C:47:ALA:O     | 2:C:50:GLU:HG2    | 2.11                     | 0.50              |
| 2:C:94:LEU:HB3   | 2:C:116:GLY:O     | 2.11                     | 0.50              |
| 2:C:971:LYS:HA   | 2:C:988:VAL:HA    | 1.93                     | 0.50              |
| 3:D:1068:LEU:HG  | 3:D:1072:ILE:HD11 | 1.94                     | 0.50              |
| 3:D:1079:LYS:HA  | 3:D:1082:ALA:HB3  | 1.93                     | 0.50              |
| 3:D:121:THR:O    | 3:D:122:GLU:C     | 2.50                     | 0.50              |
| 3:D:1375:MET:HB2 | 3:D:1376:MET:HE3  | 1.92                     | 0.50              |
| 3:D:266:GLU:HB3  | 3:D:286:VAL:CG2   | 2.42                     | 0.50              |
| 3:D:370:ALA:N    | 3:D:376:GLU:OE2   | 2.44                     | 0.50              |
| 3:D:411:THR:HG23 | 3:D:411:THR:O     | 2.12                     | 0.50              |
| 3:D:564:GLU:C    | 3:D:567:ILE:HB    | 2.31                     | 0.50              |
| 3:D:770:LEU:HD11 | 3:D:919:PHE:CD1   | 2.47                     | 0.50              |
| 3:D:829:VAL:N    | 3:D:835:SER:OG    | 2.38                     | 0.50              |
| 3:D:90:MET:HE3   | 3:D:520:LEU:HA    | 1.93                     | 0.50              |
| 5:F:203:THR:HG22 | 5:F:204:GLY:N     | 2.26                     | 0.50              |
| 5:F:287:THR:HG23 | 5:F:290:GLU:OE1   | 2.12                     | 0.50              |
| 2:C:772:ARG:HD3  | 5:F:373:LYS:CD    | 2.41                     | 0.50              |
| 5:F:98:GLU:O     | 5:F:99:GLU:C      | 2.50                     | 0.50              |
| 1:L:52:ALA:HB1   | 1:L:170:VAL:N     | 2.26                     | 0.50              |
| 1:L:5:LYS:O      | 1:L:7:LYS:N       | 2.45                     | 0.50              |
| 2:M:1007:ALA:HA  | 3:N:627:GLY:CA    | 2.41                     | 0.50              |
| 2:M:172:ILE:HG22 | 2:M:173:ASP:H     | 1.77                     | 0.50              |
| 2:M:227:PHE:CD1  | 2:M:227:PHE:N     | 2.79                     | 0.50              |
| 2:M:233:GLU:CD   | 2:M:234:ALA:H     | 2.15                     | 0.50              |
| 2:M:261:ILE:C    | 2:M:288:ARG:NH2   | 2.65                     | 0.50              |
| 2:M:303:PHE:O    | 2:M:304:LEU:C     | 2.49                     | 0.50              |
| 3:N:1276:GLU:O   | 3:N:1277:ILE:HD13 | 2.12                     | 0.50              |
| 3:N:133:ILE:HD13 | 3:N:456:MET:CE    | 2.41                     | 0.50              |
| 3:N:1488:ASP:OD1 | 3:N:1491:THR:CB   | 2.59                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:336:PHE:C    | 3:N:337:LEU:HD23  | 2.31                     | 0.50              |
| 3:N:36:THR:HG22  | 3:N:38:LYS:HE2    | 1.93                     | 0.50              |
| 3:N:41:ARG:HG3   | 3:N:41:ARG:HH11   | 1.76                     | 0.50              |
| 3:N:412:GLY:N    | 3:N:435:VAL:O     | 2.40                     | 0.50              |
| 2:M:984:GLU:HG3  | 3:N:944:THR:O     | 2.12                     | 0.50              |
| 5:P:109:GLY:O    | 5:P:112:ALA:HB3   | 2.11                     | 0.50              |
| 5:P:288:TYR:HA   | 5:P:291:ILE:HG23  | 1.92                     | 0.50              |
| 5:P:356:LYS:HD3  | 5:P:417:LYS:HZ1   | 1.76                     | 0.50              |
| 5:P:379:ARG:HH11 | 5:P:379:ARG:CB    | 2.24                     | 0.50              |
| 1:A:36:LEU:O     | 1:A:37:GLY:C      | 2.49                     | 0.50              |
| 2:C:300:ASP:CG   | 2:C:302:VAL:HB    | 2.31                     | 0.50              |
| 2:C:499:ALA:HA   | 2:C:532:MET:HE3   | 1.94                     | 0.50              |
| 2:C:394:PHE:HB3  | 2:C:632:ASN:ND2   | 2.27                     | 0.50              |
| 2:C:718:GLY:O    | 2:C:761:PHE:HE1   | 1.95                     | 0.50              |
| 2:C:722:ILE:HA   | 2:C:757:GLY:O     | 2.11                     | 0.50              |
| 2:C:807:ARG:CB   | 2:C:807:ARG:NH1   | 2.75                     | 0.50              |
| 2:C:695:LEU:CD2  | 2:C:832:LYS:HE2   | 2.42                     | 0.50              |
| 3:D:135:LEU:CD1  | 3:D:148:GLU:HB2   | 2.41                     | 0.50              |
| 3:D:1494:ALA:O   | 3:D:1497:GLU:HG2  | 2.11                     | 0.50              |
| 3:D:247:GLU:HA   | 3:D:308:LYS:NZ    | 2.25                     | 0.50              |
| 3:D:359:ALA:N    | 3:D:385:VAL:HB    | 2.27                     | 0.50              |
| 3:D:407:VAL:CG2  | 3:D:408:GLU:H     | 2.23                     | 0.50              |
| 3:D:422:ALA:H    | 3:D:427:VAL:HB    | 1.76                     | 0.50              |
| 3:D:434:ARG:NE   | 3:D:449:SER:O     | 2.45                     | 0.50              |
| 3:D:520:LEU:HD12 | 3:D:521:PRO:HD2   | 1.94                     | 0.50              |
| 3:D:676:MET:O    | 3:D:676:MET:SD    | 2.70                     | 0.50              |
| 3:D:711:LEU:C    | 3:D:713:ILE:H     | 2.13                     | 0.50              |
| 3:D:818:ARG:O    | 3:D:822:ALA:N     | 2.39                     | 0.50              |
| 2:C:987:ILE:CD1  | 3:D:948:THR:HG23  | 2.41                     | 0.50              |
| 4:E:10:PHE:C     | 4:E:12:MET:H      | 2.15                     | 0.50              |
| 5:F:231:ARG:HB3  | 5:F:233:PHE:CE2   | 2.47                     | 0.50              |
| 1:K:110:LYS:N    | 1:K:113:ASP:OD2   | 2.44                     | 0.50              |
| 1:L:68:ILE:HB    | 1:L:71:VAL:HB     | 1.94                     | 0.50              |
| 2:M:1014:SER:OG  | 2:M:1017:THR:HG23 | 2.11                     | 0.50              |
| 2:M:1086:ARG:O   | 2:M:1087:VAL:C    | 2.48                     | 0.50              |
| 2:M:1102:LEU:O   | 3:N:6:ARG:N       | 2.43                     | 0.50              |
| 2:M:139:GLN:C    | 2:M:333:ILE:HD12  | 2.32                     | 0.50              |
| 2:M:498:GLN:OE1  | 3:N:1068:LEU:HB2  | 2.12                     | 0.50              |
| 2:M:59:LYS:HD2   | 2:M:59:LYS:H      | 1.74                     | 0.50              |
| 2:M:602:GLU:CG   | 2:M:646:GLY:HA2   | 2.41                     | 0.50              |
| 2:M:691:SER:OG   | 2:M:693:GLU:HB3   | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:768:THR:HG22  | 2:M:770:GLU:HG2  | 1.93                     | 0.50              |
| 2:M:946:ARG:HH11  | 2:M:984:GLU:HB2  | 1.77                     | 0.50              |
| 3:N:1038:LEU:HD23 | 3:N:1061:PHE:HB2 | 1.94                     | 0.50              |
| 3:N:127:LEU:CD2   | 3:N:128:TYR:N    | 2.65                     | 0.50              |
| 3:N:458:ALA:HB2   | 3:N:513:ILE:HD11 | 1.90                     | 0.50              |
| 3:N:960:LYS:HE3   | 3:N:964:LEU:HD11 | 1.94                     | 0.50              |
| 1:A:215:VAL:O     | 1:A:216:GLU:C    | 2.50                     | 0.50              |
| 2:C:274:ARG:CZ    | 2:C:285:LEU:CD2  | 2.90                     | 0.50              |
| 2:C:348:LEU:N     | 2:C:378:LEU:HD13 | 2.27                     | 0.50              |
| 2:C:415:PRO:C     | 2:C:417:GLY:H    | 2.16                     | 0.50              |
| 2:C:55:GLU:HG2    | 2:C:57:GLU:N     | 2.26                     | 0.50              |
| 2:C:813:VAL:HG12  | 2:C:815:LEU:HG   | 1.94                     | 0.50              |
| 3:D:1011:PHE:HE1  | 3:D:1018:ASN:CG  | 2.15                     | 0.50              |
| 3:D:140:ALA:N     | 3:D:450:TYR:HE2  | 2.00                     | 0.50              |
| 3:D:525:ARG:HH11  | 3:D:525:ARG:HG2  | 1.77                     | 0.50              |
| 3:D:911:LEU:O     | 3:D:912:LYS:C    | 2.50                     | 0.50              |
| 1:K:1:MET:H1      | 1:K:6:LEU:CD1    | 2.21                     | 0.50              |
| 1:K:90:LEU:HB2    | 1:K:119:ASP:HB3  | 1.94                     | 0.50              |
| 1:L:79:ILE:CA     | 1:L:82:LEU:HG    | 2.40                     | 0.50              |
| 2:M:1032:PHE:CZ   | 2:M:1036:GLU:HB3 | 2.47                     | 0.50              |
| 2:M:193:LEU:HD21  | 2:M:307:LEU:HD22 | 1.92                     | 0.50              |
| 2:M:509:ALA:O     | 2:M:510:ALA:HB2  | 2.10                     | 0.50              |
| 2:M:631:SER:C     | 2:M:634:GLY:H    | 2.14                     | 0.50              |
| 2:M:690:ILE:N     | 2:M:851:LYS:O    | 2.45                     | 0.50              |
| 2:M:861:LEU:CB    | 2:M:862:PRO:HD2  | 2.40                     | 0.50              |
| 2:M:911:GLU:HB2   | 2:M:912:PRO:HD3  | 1.92                     | 0.50              |
| 3:N:957:PRO:CG    | 3:N:1007:VAL:HA  | 2.41                     | 0.50              |
| 3:N:1208:ASP:O    | 3:N:1209:LEU:CB  | 2.60                     | 0.50              |
| 3:N:137:PRO:CG    | 3:N:138:LYS:N    | 2.74                     | 0.50              |
| 3:N:324:ALA:CB    | 3:N:331:VAL:HG11 | 2.42                     | 0.50              |
| 3:N:411:THR:HA    | 3:N:435:VAL:O    | 2.12                     | 0.50              |
| 3:N:477:LEU:O     | 3:N:481:MET:N    | 2.44                     | 0.50              |
| 3:N:530:VAL:HG23  | 3:N:531:ASP:N    | 2.24                     | 0.50              |
| 3:N:921:ARG:C     | 3:N:922:LEU:HD23 | 2.32                     | 0.50              |
| 5:P:151:LEU:HB2   | 5:P:155:THR:CB   | 2.42                     | 0.50              |
| 5:P:181:GLU:O     | 5:P:184:ARG:HB3  | 2.11                     | 0.50              |
| 5:P:269:ASN:O     | 5:P:270:LYS:C    | 2.50                     | 0.50              |
| 5:P:355:GLU:HA    | 5:P:358:LEU:HB3  | 1.93                     | 0.50              |
| 5:P:79:ASP:O      | 5:P:79:ASP:OD1   | 2.29                     | 0.50              |
| 3:N:572:ARG:HH12  | 5:P:84:TYR:CA    | 2.24                     | 0.50              |
| 1:A:98:THR:CG2    | 1:A:141:GLU:HB3  | 2.42                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:15:THR:CB     | 1:A:21:GLY:HA3   | 2.39                     | 0.50              |
| 1:A:38:ASN:O      | 1:A:39:PRO:C     | 2.49                     | 0.50              |
| 1:B:182:GLU:HG3   | 1:B:194:LYS:HD3  | 1.94                     | 0.50              |
| 2:C:102:HIS:O     | 2:C:105:THR:N    | 2.44                     | 0.50              |
| 2:C:230:ARG:HG2   | 2:C:230:ARG:O    | 2.11                     | 0.50              |
| 2:C:141:HIS:NE2   | 2:C:332:ARG:HB3  | 2.27                     | 0.50              |
| 2:C:389:SER:HB3   | 2:C:392:SER:HB3  | 1.94                     | 0.50              |
| 2:C:601:GLY:HA3   | 2:C:614:ARG:O    | 2.12                     | 0.50              |
| 2:C:689:VAL:O     | 2:C:690:ILE:HD13 | 2.12                     | 0.50              |
| 2:C:910:LYS:HE3   | 2:C:912:PRO:HG2  | 1.94                     | 0.50              |
| 3:D:1031:ASN:HB2  | 3:D:1032:PRO:CD  | 2.40                     | 0.50              |
| 3:D:1360:GLY:O    | 3:D:1362:LYS:HE2 | 2.12                     | 0.50              |
| 3:D:1363:LEU:HD23 | 3:D:1364:HIS:N   | 2.27                     | 0.50              |
| 3:D:192:ALA:O     | 3:D:193:PRO:C    | 2.48                     | 0.50              |
| 3:D:291:LEU:HB3   | 3:D:294:HIS:HB2  | 1.94                     | 0.50              |
| 3:D:238:PRO:CD    | 3:D:318:ARG:HA   | 2.42                     | 0.50              |
| 3:D:397:LYS:HE3   | 3:D:448:GLU:CD   | 2.32                     | 0.50              |
| 3:D:402:PRO:HA    | 3:D:443:VAL:HA   | 1.94                     | 0.50              |
| 3:D:500:ARG:O     | 3:D:504:ASP:N    | 2.33                     | 0.50              |
| 3:D:674:ARG:HG3   | 3:D:674:ARG:NH1  | 2.27                     | 0.50              |
| 3:D:710:ARG:C     | 3:D:712:GLY:H    | 2.15                     | 0.50              |
| 3:D:757:ALA:O     | 3:D:758:GLU:C    | 2.49                     | 0.50              |
| 5:F:372:ARG:CG    | 5:F:378:GLY:O    | 2.55                     | 0.50              |
| 1:K:64:GLU:CA     | 1:K:165:ILE:HD13 | 2.42                     | 0.50              |
| 2:M:1004:LYS:HB3  | 2:M:1006:HIS:CE1 | 2.47                     | 0.50              |
| 2:M:1036:GLU:CD   | 2:M:1036:GLU:H   | 2.14                     | 0.50              |
| 2:M:1042:ALA:HB3  | 3:N:710:ARG:HB2  | 1.94                     | 0.50              |
| 2:M:1048:THR:HA   | 3:N:755:ALA:HB1  | 1.94                     | 0.50              |
| 2:M:145:GLY:HA3   | 2:M:276:LYS:HD2  | 1.93                     | 0.50              |
| 2:M:405:ARG:HH22  | 2:M:409:ARG:CZ   | 2.25                     | 0.50              |
| 2:M:41:ASN:O      | 2:M:42:VAL:C     | 2.50                     | 0.50              |
| 2:M:455:LEU:HD12  | 2:M:456:ALA:H    | 1.77                     | 0.50              |
| 2:M:41:ASN:O      | 2:M:46:ALA:CB    | 2.60                     | 0.50              |
| 2:M:807:ARG:CB    | 2:M:807:ARG:CZ   | 2.90                     | 0.50              |
| 2:M:833:LEU:CD1   | 2:M:837:ASP:HB2  | 2.42                     | 0.50              |
| 2:M:948:GLU:CB    | 2:M:953:VAL:HG23 | 2.42                     | 0.50              |
| 3:N:1229:ILE:C    | 3:N:1232:PRO:HD2 | 2.32                     | 0.50              |
| 3:N:1269:LYS:C    | 3:N:1271:LYS:N   | 2.66                     | 0.50              |
| 3:N:160:GLU:O     | 3:N:164:GLY:O    | 2.29                     | 0.50              |
| 3:N:174:GLY:HA2   | 3:N:389:GLU:CD   | 2.32                     | 0.50              |
| 3:N:36:THR:CB     | 3:N:38:LYS:HG2   | 2.24                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:586:ARG:O     | 3:N:587:ARG:CG    | 2.60                     | 0.50              |
| 3:N:592:THR:CG2   | 3:N:598:ARG:HH12  | 2.24                     | 0.50              |
| 3:N:60:CYS:CB     | 3:N:62:LYS:HE2    | 2.36                     | 0.50              |
| 3:N:729:HIS:CG    | 3:N:730:PRO:HD2   | 2.47                     | 0.50              |
| 1:B:171:PHE:O     | 1:B:172:SER:C     | 2.50                     | 0.49              |
| 1:B:99:LEU:HB3    | 1:B:114:PHE:CD2   | 2.47                     | 0.49              |
| 2:C:65:VAL:HB     | 2:C:101:ILE:HB    | 1.94                     | 0.49              |
| 2:C:312:ALA:O     | 2:C:318:PRO:HB2   | 2.12                     | 0.49              |
| 2:C:504:GLU:OE2   | 2:C:507:ARG:HD3   | 2.12                     | 0.49              |
| 2:C:721:ARG:O     | 2:C:758:ARG:HA    | 2.13                     | 0.49              |
| 2:C:862:PRO:C     | 2:C:864:GLY:H     | 2.15                     | 0.49              |
| 3:D:1460:ILE:HG13 | 3:D:1461:GLY:N    | 2.26                     | 0.49              |
| 3:D:297:ILE:HG23  | 3:D:298:VAL:H     | 1.76                     | 0.49              |
| 3:D:625:TYR:CD1   | 3:D:625:TYR:N     | 2.80                     | 0.49              |
| 3:D:673:ALA:O     | 3:D:676:MET:HB3   | 2.11                     | 0.49              |
| 3:D:932:ASP:O     | 3:D:935:LYS:HB3   | 2.11                     | 0.49              |
| 3:D:965:GLU:CD    | 3:D:965:GLU:C     | 2.71                     | 0.49              |
| 5:F:127:ILE:O     | 5:F:130:VAL:HB    | 2.11                     | 0.49              |
| 5:F:282:LEU:C     | 5:F:284:ARG:H     | 2.15                     | 0.49              |
| 5:F:320:PRO:HA    | 5:F:327:SER:O     | 2.12                     | 0.49              |
| 2:C:1015:LEU:CB   | 5:F:333:ILE:HG22  | 2.42                     | 0.49              |
| 5:F:82:ARG:HH11   | 5:F:82:ARG:HG3    | 1.76                     | 0.49              |
| 2:M:1008:ARG:O    | 3:N:652:LEU:HD23  | 2.12                     | 0.49              |
| 2:M:101:ILE:CG2   | 2:M:102:HIS:N     | 2.67                     | 0.49              |
| 2:M:170:PRO:HD2   | 2:M:263:ASP:O     | 2.12                     | 0.49              |
| 2:M:430:VAL:HA    | 2:M:434:HIS:CD2   | 2.47                     | 0.49              |
| 2:M:496:ILE:HA    | 2:M:531:PHE:O     | 2.12                     | 0.49              |
| 2:M:606:VAL:HG12  | 2:M:611:ILE:CG2   | 2.39                     | 0.49              |
| 2:M:689:VAL:HG22  | 2:M:870:ILE:HB    | 1.93                     | 0.49              |
| 2:M:861:LEU:HD23  | 2:M:861:LEU:N     | 2.26                     | 0.49              |
| 3:N:1155:VAL:O    | 3:N:1158:VAL:HG12 | 2.12                     | 0.49              |
| 3:N:1495:ILE:CG2  | 3:N:1496:GLU:H    | 2.22                     | 0.49              |
| 3:N:29:PRO:HG3    | 3:N:548:ILE:CB    | 2.41                     | 0.49              |
| 3:N:393:ILE:HG22  | 3:N:394:LEU:N     | 2.27                     | 0.49              |
| 3:N:443:VAL:CG1   | 3:N:444:VAL:N     | 2.75                     | 0.49              |
| 5:P:146:GLY:N     | 5:P:149:GLU:HB2   | 2.27                     | 0.49              |
| 5:P:194:LEU:HD13  | 5:P:194:LEU:O     | 2.12                     | 0.49              |
| 1:A:151:VAL:HG13  | 1:A:155:LYS:HG2   | 1.94                     | 0.49              |
| 1:A:217:ILE:HG22  | 1:A:221:HIS:CD2   | 2.47                     | 0.49              |
| 1:B:151:VAL:HG21  | 1:B:171:PHE:CE1   | 2.48                     | 0.49              |
| 1:B:58:ILE:HD13   | 1:B:58:ILE:C      | 2.32                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:273:GLY:HA2   | 2:C:276:LYS:HG3   | 1.94                     | 0.49              |
| 2:C:41:ASN:OD1    | 2:C:46:ALA:HA     | 2.13                     | 0.49              |
| 2:C:494:TYR:HB3   | 2:C:530:GLU:OE2   | 2.12                     | 0.49              |
| 2:C:579:VAL:HA    | 2:C:901:TYR:O     | 2.12                     | 0.49              |
| 2:C:599:GLU:HB3   | 2:C:615:TYR:CE2   | 2.47                     | 0.49              |
| 2:C:731:GLU:O     | 2:C:734:LEU:N     | 2.42                     | 0.49              |
| 3:D:1335:LEU:HD12 | 3:D:1335:LEU:O    | 2.12                     | 0.49              |
| 3:D:257:GLY:CA    | 3:D:274:ARG:HA    | 2.28                     | 0.49              |
| 3:D:171:LEU:CD1   | 3:D:390:PRO:HB2   | 2.41                     | 0.49              |
| 3:D:560:GLN:HA    | 3:D:560:GLN:OE1   | 2.11                     | 0.49              |
| 3:D:598:ARG:HH11  | 3:D:598:ARG:HG2   | 1.76                     | 0.49              |
| 3:D:657:LEU:O     | 3:D:658:LEU:C     | 2.50                     | 0.49              |
| 4:E:49:GLN:HG3    | 4:E:54:LEU:HD23   | 1.93                     | 0.49              |
| 4:E:67:GLU:O      | 4:E:70:THR:O      | 2.30                     | 0.49              |
| 5:F:145:PRO:HB3   | 5:F:152:ASP:OD2   | 2.11                     | 0.49              |
| 5:F:288:TYR:HB3   | 5:F:301:ALA:CB    | 2.42                     | 0.49              |
| 1:K:29:GLU:O      | 1:K:30:ARG:C      | 2.51                     | 0.49              |
| 1:K:44:LEU:CD2    | 1:K:214:ALA:HB2   | 2.42                     | 0.49              |
| 1:K:11:PHE:CE2    | 1:L:225:PHE:O     | 2.65                     | 0.49              |
| 2:M:1012:PRO:HD2  | 2:M:1021:LEU:O    | 2.12                     | 0.49              |
| 2:M:211:LEU:C     | 2:M:213:ALA:N     | 2.64                     | 0.49              |
| 2:M:313:LEU:C     | 2:M:315:ALA:N     | 2.65                     | 0.49              |
| 2:M:754:ILE:HG12  | 2:M:791:ARG:HD2   | 1.93                     | 0.49              |
| 3:N:1117:TYR:HA   | 3:N:1193:THR:HG21 | 1.94                     | 0.49              |
| 3:N:1229:ILE:O    | 3:N:1232:PRO:HD2  | 2.11                     | 0.49              |
| 3:N:1311:LEU:HD21 | 3:N:1313:VAL:O    | 2.12                     | 0.49              |
| 3:N:1130:ARG:NH2  | 3:N:1323:GLN:NE2  | 2.57                     | 0.49              |
| 3:N:1364:HIS:ND1  | 3:N:1366:LYS:HG3  | 2.27                     | 0.49              |
| 3:N:414:ARG:O     | 3:N:415:VAL:HG13  | 2.11                     | 0.49              |
| 3:N:47:GLU:CB     | 3:N:51:GLY:O      | 2.60                     | 0.49              |
| 3:N:671:LYS:O     | 3:N:674:ARG:HB2   | 2.11                     | 0.49              |
| 3:N:703:ASN:HD22  | 3:N:704:ARG:N     | 2.11                     | 0.49              |
| 4:O:46:PRO:O      | 4:O:57:ASP:N      | 2.38                     | 0.49              |
| 5:P:349:LEU:HA    | 5:P:352:GLU:CD    | 2.33                     | 0.49              |
| 5:P:402:ASN:HD22  | 5:P:402:ASN:N     | 2.09                     | 0.49              |
| 1:B:6:LEU:C       | 1:B:8:ALA:H       | 2.15                     | 0.49              |
| 2:C:1039:ALA:HA   | 3:D:1227:GLN:NE2  | 2.27                     | 0.49              |
| 2:C:157:ARG:CG    | 2:C:158:TYR:H     | 2.13                     | 0.49              |
| 2:C:332:ARG:HG2   | 2:C:333:ILE:N     | 2.27                     | 0.49              |
| 2:C:115:LEU:CD1   | 2:C:373:VAL:CG1   | 2.73                     | 0.49              |
| 2:C:543:ASN:HA    | 2:C:546:LEU:CD1   | 2.41                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:757:GLY:HA2   | 2:C:789:SER:HB3   | 1.93                     | 0.49              |
| 3:D:1084:THR:HG23 | 3:D:1085:ALA:H    | 1.76                     | 0.49              |
| 3:D:155:ASP:O     | 3:D:158:TYR:N     | 2.45                     | 0.49              |
| 3:D:227:LEU:HG    | 3:D:326:GLU:OE1   | 2.12                     | 0.49              |
| 3:D:243:ALA:HB3   | 3:D:311:LEU:CD1   | 2.34                     | 0.49              |
| 3:D:248:PRO:HB3   | 3:D:308:LYS:NZ    | 2.26                     | 0.49              |
| 3:D:59:ALA:HB3    | 3:D:76:CYS:CB     | 2.42                     | 0.49              |
| 3:D:605:ASP:OD1   | 3:D:605:ASP:N     | 2.45                     | 0.49              |
| 3:D:605:ASP:O     | 3:D:609:GLY:HA2   | 2.12                     | 0.49              |
| 3:D:660:LYS:O     | 3:D:663:GLU:HB2   | 2.12                     | 0.49              |
| 3:D:853:VAL:O     | 3:D:856:GLY:N     | 2.41                     | 0.49              |
| 3:D:932:ASP:HA    | 3:D:935:LYS:HE2   | 1.94                     | 0.49              |
| 5:F:225:GLU:OE1   | 5:F:226:LYS:NZ    | 2.44                     | 0.49              |
| 5:F:271:LEU:CD1   | 5:F:307:THR:HG21  | 2.40                     | 0.49              |
| 1:K:199:ILE:HG21  | 1:K:207:PRO:HA    | 1.94                     | 0.49              |
| 2:M:1085:PHE:O    | 2:M:1089:VAL:HG23 | 2.12                     | 0.49              |
| 2:M:193:LEU:O     | 2:M:195:LEU:N     | 2.45                     | 0.49              |
| 2:M:18:LEU:C      | 2:M:20:GLU:N      | 2.65                     | 0.49              |
| 2:M:317:VAL:HG13  | 2:M:320:HIS:CE1   | 2.47                     | 0.49              |
| 2:M:396:ASP:O     | 2:M:403:SER:CA    | 2.60                     | 0.49              |
| 2:M:486:MET:HG2   | 2:M:487:THR:O     | 2.11                     | 0.49              |
| 2:M:504:GLU:OE2   | 2:M:507:ARG:HD3   | 2.12                     | 0.49              |
| 2:M:591:SER:O     | 2:M:592:LEU:HB2   | 2.12                     | 0.49              |
| 2:M:611:ILE:HD11  | 2:M:641:PRO:HB3   | 1.93                     | 0.49              |
| 2:M:676:ILE:CG1   | 2:M:873:PRO:HG3   | 2.40                     | 0.49              |
| 2:M:728:HIS:CG    | 2:M:729:LEU:N     | 2.80                     | 0.49              |
| 2:M:815:LEU:HD21  | 2:M:822:VAL:HG22  | 1.92                     | 0.49              |
| 3:N:1117:TYR:HD1  | 3:N:1118:ILE:O    | 1.95                     | 0.49              |
| 3:N:1418:LYS:O    | 3:N:1420:LEU:HD13 | 2.11                     | 0.49              |
| 3:N:302:GLN:N     | 3:N:303:PRO:CD    | 2.75                     | 0.49              |
| 3:N:42:ASP:OD1    | 3:N:48:ARG:NH2    | 2.45                     | 0.49              |
| 3:N:483:HIS:CB    | 3:N:484:PRO:CD    | 2.79                     | 0.49              |
| 3:N:712:GLY:O     | 3:N:713:ILE:HG13  | 2.12                     | 0.49              |
| 3:N:758:GLU:HG2   | 4:O:20:THR:HG21   | 1.94                     | 0.49              |
| 1:B:158:ILE:C     | 1:B:159:LYS:HG3   | 2.33                     | 0.49              |
| 1:B:219:ARG:HG2   | 1:B:219:ARG:NH1   | 2.23                     | 0.49              |
| 2:C:178:PRO:HB2   | 2:C:220:GLY:HA3   | 1.94                     | 0.49              |
| 2:C:617:ASP:OD2   | 2:C:619:ARG:HG3   | 2.13                     | 0.49              |
| 2:C:594:ALA:HB1   | 2:C:654:LEU:HD11  | 1.94                     | 0.49              |
| 3:D:1007:VAL:O    | 3:D:1010:ASN:HB3  | 2.11                     | 0.49              |
| 3:D:1066:THR:O    | 3:D:1070:TYR:N    | 2.39                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1293:PHE:HD1 | 3:D:1302:GLU:HA   | 1.75                     | 0.49              |
| 3:D:1379:VAL:O   | 3:D:1393:GLN:N    | 2.44                     | 0.49              |
| 3:D:1464:GLU:HG2 | 3:D:1465:ASN:H    | 1.77                     | 0.49              |
| 3:D:358:GLY:HA2  | 3:D:385:VAL:C     | 2.32                     | 0.49              |
| 3:D:500:ARG:O    | 3:D:504:ASP:HB2   | 2.12                     | 0.49              |
| 3:D:960:LYS:HG2  | 3:D:964:LEU:HD12  | 1.93                     | 0.49              |
| 5:F:112:ALA:O    | 5:F:116:LEU:HG    | 2.12                     | 0.49              |
| 5:F:135:ILE:HD12 | 5:F:181:GLU:HB3   | 1.95                     | 0.49              |
| 1:K:89:PHE:CB    | 1:K:146:ARG:HH21  | 2.23                     | 0.49              |
| 1:K:173:PRO:HG3  | 1:K:205:VAL:HG21  | 1.92                     | 0.49              |
| 1:L:134:GLU:C    | 1:L:136:GLY:H     | 2.16                     | 0.49              |
| 2:M:1061:GLU:HA  | 2:M:1064:ASN:HD22 | 1.78                     | 0.49              |
| 2:M:146:VAL:HG22 | 2:M:162:ILE:CG1   | 2.36                     | 0.49              |
| 2:M:268:ASP:O    | 2:M:288:ARG:HD2   | 2.12                     | 0.49              |
| 2:M:355:VAL:HA   | 2:M:358:ARG:CG    | 2.41                     | 0.49              |
| 2:M:382:ILE:O    | 2:M:385:PHE:HB3   | 2.12                     | 0.49              |
| 2:M:426:ASP:O    | 2:M:429:ASP:HB2   | 2.12                     | 0.49              |
| 2:M:543:ASN:HA   | 2:M:546:LEU:CD1   | 2.39                     | 0.49              |
| 2:M:569:VAL:HG23 | 2:M:570:PRO:HD2   | 1.95                     | 0.49              |
| 2:M:730:SER:OG   | 2:M:731:GLU:N     | 2.45                     | 0.49              |
| 2:M:742:VAL:HG12 | 2:M:743:VAL:N     | 2.27                     | 0.49              |
| 2:M:800:VAL:HG12 | 2:M:801:VAL:H     | 1.78                     | 0.49              |
| 2:M:894:GLY:HA2  | 2:M:901:TYR:OH    | 2.11                     | 0.49              |
| 3:N:1165:TYR:HE2 | 3:N:1206:GLY:HA2  | 1.77                     | 0.49              |
| 3:N:1166:LEU:HA  | 3:N:1170:ASP:OD2  | 2.12                     | 0.49              |
| 3:N:1306:PRO:HB2 | 3:N:1308:GLU:HG3  | 1.93                     | 0.49              |
| 3:N:169:TYR:O    | 3:N:392:SER:HB3   | 2.13                     | 0.49              |
| 3:N:210:ARG:HB3  | 3:N:388:HIS:HB2   | 1.94                     | 0.49              |
| 3:N:413:ASP:O    | 3:N:435:VAL:N     | 2.45                     | 0.49              |
| 5:P:135:ILE:C    | 5:P:137:GLY:H     | 2.15                     | 0.49              |
| 5:P:152:ASP:HA   | 5:P:156:VAL:HG11  | 1.94                     | 0.49              |
| 5:P:156:VAL:HG23 | 5:P:157:GLU:H     | 1.77                     | 0.49              |
| 5:P:367:MET:CB   | 5:P:370:LYS:HE2   | 2.38                     | 0.49              |
| 1:A:103:ALA:O    | 1:A:104:GLU:HB2   | 2.11                     | 0.49              |
| 1:A:170:VAL:O    | 1:A:170:VAL:HG23  | 2.13                     | 0.49              |
| 1:A:222:LEU:HA   | 1:A:225:PHE:CE1   | 2.47                     | 0.49              |
| 1:B:182:GLU:CG   | 1:B:194:LYS:HD3   | 2.42                     | 0.49              |
| 1:B:5:LYS:HZ3    | 1:B:189:ARG:CZ    | 2.25                     | 0.49              |
| 1:B:64:GLU:O     | 1:B:76:VAL:HG23   | 2.13                     | 0.49              |
| 2:C:176:VAL:HG12 | 2:C:182:VAL:HA    | 1.94                     | 0.49              |
| 2:C:214:TYR:OH   | 2:C:308:ARG:HB2   | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:36:PRO:HG2   | 2:C:38:LYS:HB3   | 1.94                     | 0.49              |
| 2:C:630:ARG:HD2  | 2:C:705:ILE:HB   | 1.93                     | 0.49              |
| 2:C:896:PHE:C    | 2:C:898:GLY:N    | 2.66                     | 0.49              |
| 3:D:775:GLY:HA2  | 3:D:1209:LEU:O   | 2.12                     | 0.49              |
| 3:D:172:PRO:HB2  | 3:D:175:VAL:HG23 | 1.93                     | 0.49              |
| 3:D:15:PRO:HA    | 3:D:18:ILE:HD12  | 1.94                     | 0.49              |
| 3:D:206:ARG:HB3  | 3:D:207:PHE:CD1  | 2.48                     | 0.49              |
| 3:D:258:VAL:HG23 | 3:D:273:ARG:O    | 2.13                     | 0.49              |
| 3:D:28:LYS:HG2   | 3:D:42:ASP:O     | 2.13                     | 0.49              |
| 3:D:32:ILE:CG2   | 3:D:37:LEU:HA    | 2.42                     | 0.49              |
| 3:D:558:LEU:C    | 3:D:560:GLN:N    | 2.64                     | 0.49              |
| 3:D:678:GLU:HG3  | 3:D:679:ARG:CG   | 2.38                     | 0.49              |
| 5:F:209:PHE:O    | 5:F:212:LEU:HB2  | 2.13                     | 0.49              |
| 1:K:9:PRO:HA     | 1:K:26:GLU:O     | 2.12                     | 0.49              |
| 2:M:1050:GLN:O   | 2:M:1053:LEU:N   | 2.40                     | 0.49              |
| 2:M:297:GLU:H    | 2:M:297:GLU:CD   | 2.15                     | 0.49              |
| 2:M:428:ARG:NH2  | 2:M:451:LEU:HD11 | 2.27                     | 0.49              |
| 2:M:512:ARG:HD2  | 2:M:523:ILE:CG1  | 2.39                     | 0.49              |
| 2:M:541:SER:O    | 2:M:544:THR:HB   | 2.13                     | 0.49              |
| 2:M:63:GLY:H     | 2:M:103:LYS:CB   | 2.26                     | 0.49              |
| 2:M:926:PHE:O    | 2:M:927:GLY:C    | 2.50                     | 0.49              |
| 3:N:1155:VAL:O   | 3:N:1158:VAL:CG1 | 2.60                     | 0.49              |
| 3:N:1167:SER:N   | 3:N:1170:ASP:OD2 | 2.46                     | 0.49              |
| 3:N:1350:GLU:O   | 3:N:1354:LYS:HG3 | 2.12                     | 0.49              |
| 3:N:1487:VAL:O   | 4:O:74:VAL:HG22  | 2.12                     | 0.49              |
| 3:N:188:GLY:H    | 3:N:197:SER:C    | 2.15                     | 0.49              |
| 3:N:323:GLU:CB   | 3:N:334:THR:HB   | 2.39                     | 0.49              |
| 5:P:111:GLU:CG   | 5:P:114:LYS:HZ2  | 2.23                     | 0.49              |
| 5:P:156:VAL:O    | 5:P:159:ILE:HB   | 2.12                     | 0.49              |
| 5:P:370:LYS:HA   | 5:P:374:GLY:CA   | 2.42                     | 0.49              |
| 5:P:367:MET:HE1  | 5:P:371:LEU:HD21 | 1.94                     | 0.49              |
| 1:A:111:ALA:C    | 1:A:113:ASP:N    | 2.65                     | 0.49              |
| 1:A:124:ASN:HB2  | 1:A:127:LEU:CB   | 2.43                     | 0.49              |
| 1:A:150:TYR:HA   | 1:A:169:ALA:O    | 2.12                     | 0.49              |
| 1:A:177:VAL:HG12 | 1:A:178:ALA:N    | 2.27                     | 0.49              |
| 1:A:222:LEU:HD12 | 1:B:219:ARG:HA   | 1.94                     | 0.49              |
| 2:C:471:TYR:CE2  | 2:C:496:ILE:HG21 | 2.48                     | 0.49              |
| 2:C:73:LEU:O     | 2:C:73:LEU:HD12  | 2.11                     | 0.49              |
| 2:C:96:ALA:HB3   | 2:C:113:VAL:HG23 | 1.95                     | 0.49              |
| 3:D:254:GLU:CD   | 3:D:299:GLU:O    | 2.51                     | 0.49              |
| 3:D:912:LYS:O    | 3:D:915:VAL:HB   | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1488:ASP:HA   | 4:E:73:LEU:HD13  | 1.94                     | 0.49              |
| 5:F:118:GLU:C     | 5:F:120:THR:N    | 2.63                     | 0.49              |
| 5:F:291:ILE:O     | 5:F:295:MET:N    | 2.33                     | 0.49              |
| 5:F:408:LEU:O     | 5:F:411:HIS:N    | 2.42                     | 0.49              |
| 1:K:122:ILE:CG2   | 1:K:123:MET:N    | 2.76                     | 0.49              |
| 2:M:63:GLY:O      | 2:M:102:HIS:HA   | 2.13                     | 0.49              |
| 2:M:1060:ILE:HG13 | 2:M:1083:GLU:HG3 | 1.94                     | 0.49              |
| 2:M:37:GLU:CG     | 2:M:71:TYR:HE2   | 2.23                     | 0.49              |
| 2:M:410:ILE:N     | 2:M:410:ILE:HD12 | 2.28                     | 0.49              |
| 2:M:431:HIS:ND1   | 2:M:432:ARG:HG2  | 2.28                     | 0.49              |
| 2:M:65:VAL:HG12   | 2:M:66:LEU:N     | 2.27                     | 0.49              |
| 2:M:971:LYS:HZ1   | 3:N:950:GLY:HA3  | 1.78                     | 0.49              |
| 3:N:1092:GLY:O    | 3:N:1093:TYR:C   | 2.50                     | 0.49              |
| 3:N:1472:ILE:HD13 | 3:N:1473:PRO:HD3 | 1.93                     | 0.49              |
| 3:N:520:LEU:HD12  | 3:N:521:PRO:HD2  | 1.95                     | 0.49              |
| 3:N:789:LEU:HG    | 3:N:938:GLY:HA2  | 1.95                     | 0.49              |
| 3:N:812:ALA:O     | 3:N:814:ALA:N    | 2.45                     | 0.49              |
| 3:N:959:GLU:N     | 3:N:959:GLU:CD   | 2.65                     | 0.49              |
| 5:P:107:GLU:OE1   | 5:P:230:LYS:HE3  | 2.11                     | 0.49              |
| 5:P:151:LEU:HB2   | 5:P:155:THR:HB   | 1.94                     | 0.49              |
| 5:P:216:GLY:CA    | 5:P:243:ILE:HG23 | 2.42                     | 0.49              |
| 1:A:29:GLU:O      | 1:A:193:ASP:OD2  | 2.30                     | 0.49              |
| 1:A:68:ILE:HG23   | 1:A:69:PRO:HD2   | 1.95                     | 0.49              |
| 1:A:76:VAL:O      | 1:A:77:GLU:C     | 2.51                     | 0.49              |
| 2:C:1102:LEU:HD11 | 3:D:9:ARG:HB2    | 1.95                     | 0.49              |
| 2:C:175:GLU:HG2   | 2:C:176:VAL:H    | 1.76                     | 0.49              |
| 2:C:138:SER:O     | 2:C:410:ILE:HA   | 2.12                     | 0.49              |
| 3:D:1160:LEU:O    | 3:D:1161:GLU:C   | 2.50                     | 0.49              |
| 3:D:1398:TRP:O    | 3:D:1402:ALA:HB3 | 2.12                     | 0.49              |
| 3:D:1434:TRP:CZ3  | 3:D:1457:ASP:HB2 | 2.48                     | 0.49              |
| 3:D:1470:ARG:HG2  | 3:D:1471:LEU:N   | 2.28                     | 0.49              |
| 3:D:33:ASN:O      | 3:D:37:LEU:N     | 2.46                     | 0.49              |
| 3:D:509:PRO:HG2   | 3:D:510:GLU:OE2  | 2.13                     | 0.49              |
| 3:D:814:ALA:O     | 3:D:818:ARG:HG3  | 2.11                     | 0.49              |
| 4:E:55:PHE:N      | 4:E:55:PHE:CD1   | 2.81                     | 0.49              |
| 5:F:300:ASP:CG    | 5:F:302:LYS:HE3  | 2.32                     | 0.49              |
| 5:F:321:ILE:CG2   | 5:F:322:GLY:H    | 2.26                     | 0.49              |
| 5:F:386:VAL:CG1   | 5:F:394:ARG:N    | 2.76                     | 0.49              |
| 1:L:85:LEU:HD11   | 1:L:87:VAL:HG13  | 1.94                     | 0.49              |
| 2:M:1114:GLY:C    | 2:M:1116:ALA:N   | 2.65                     | 0.49              |
| 2:M:322:VAL:HG12  | 2:M:323:ASP:N    | 2.20                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:650:ARG:CA    | 2:M:650:ARG:HE   | 2.22                     | 0.49              |
| 2:M:869:VAL:CG2   | 2:M:870:ILE:N    | 2.76                     | 0.49              |
| 2:M:946:ARG:NH1   | 2:M:984:GLU:HB2  | 2.28                     | 0.49              |
| 3:N:1095:THR:O    | 3:N:1096:ARG:C   | 2.51                     | 0.49              |
| 3:N:1112:CYS:N    | 3:N:1201:CYS:HB2 | 2.28                     | 0.49              |
| 3:N:135:LEU:H     | 3:N:135:LEU:HD23 | 1.75                     | 0.49              |
| 3:N:1447:LEU:O    | 3:N:1448:THR:C   | 2.49                     | 0.49              |
| 3:N:154:THR:HG23  | 3:N:157:GLU:H    | 1.77                     | 0.49              |
| 3:N:16:GLU:N      | 3:N:16:GLU:CD    | 2.61                     | 0.49              |
| 3:N:207:PHE:CB    | 3:N:391:ALA:HB3  | 2.41                     | 0.49              |
| 3:N:18:ILE:HG21   | 3:N:518:PRO:HG3  | 1.95                     | 0.49              |
| 5:P:132:ARG:CZ    | 5:P:184:ARG:HH12 | 2.25                     | 0.49              |
| 5:P:206:GLY:O     | 5:P:207:LEU:HB2  | 2.11                     | 0.49              |
| 5:P:288:TYR:CA    | 5:P:291:ILE:HG23 | 2.42                     | 0.49              |
| 5:P:302:LYS:O     | 5:P:306:GLU:OE2  | 2.30                     | 0.49              |
| 5:P:383:LEU:HD23  | 5:P:394:ARG:HD3  | 1.93                     | 0.49              |
| 5:P:416:ARG:HD2   | 5:P:419:ARG:CG   | 2.40                     | 0.49              |
| 1:A:63:HIS:HB2    | 2:C:799:ILE:HD11 | 1.93                     | 0.49              |
| 1:B:240:LYS:HD2   | 1:B:240:LYS:N    | 2.28                     | 0.49              |
| 2:C:428:ARG:NH2   | 2:C:451:LEU:HD11 | 2.28                     | 0.49              |
| 2:C:630:ARG:HG3   | 2:C:631:SER:N    | 2.27                     | 0.49              |
| 2:C:691:SER:HB2   | 2:C:868:ASP:HA   | 1.93                     | 0.49              |
| 2:C:731:GLU:C     | 2:C:733:ALA:N    | 2.64                     | 0.49              |
| 2:C:918:LEU:CD1   | 2:C:968:LEU:HA   | 2.42                     | 0.49              |
| 3:D:1078:ARG:O    | 3:D:1080:GLY:N   | 2.46                     | 0.49              |
| 3:D:1207:TYR:HA   | 3:D:1213:ARG:O   | 2.11                     | 0.49              |
| 3:D:1253:THR:HG22 | 3:D:1254:GLN:N   | 2.28                     | 0.49              |
| 3:D:1339:LYS:HB3  | 3:D:1343:ALA:CB  | 2.41                     | 0.49              |
| 3:D:16:GLU:N      | 3:D:16:GLU:OE1   | 2.46                     | 0.49              |
| 3:D:248:PRO:CA    | 3:D:308:LYS:NZ   | 2.73                     | 0.49              |
| 3:D:277:GLU:HG3   | 3:D:278:PRO:N    | 2.27                     | 0.49              |
| 3:D:408:GLU:CD    | 3:D:421:LEU:HG   | 2.32                     | 0.49              |
| 3:D:68:PHE:HZ     | 5:F:376:ILE:HG12 | 1.77                     | 0.49              |
| 3:D:736:PHE:O     | 3:D:737:ASN:C    | 2.51                     | 0.49              |
| 3:D:806:PHE:CZ    | 3:D:816:HIS:CE1  | 3.01                     | 0.49              |
| 3:D:844:ALA:N     | 3:D:848:GLU:OE1  | 2.45                     | 0.49              |
| 3:D:926:LYS:HE2   | 3:D:929:ARG:NH1  | 2.28                     | 0.49              |
| 3:D:785:ILE:HG23  | 3:D:938:GLY:HA3  | 1.95                     | 0.49              |
| 5:F:304:VAL:HG12  | 5:F:308:LEU:HD21 | 1.94                     | 0.49              |
| 5:F:381:HIS:N     | 5:F:385:GLU:CD   | 2.66                     | 0.49              |
| 5:F:393:THR:CG2   | 5:F:394:ARG:N    | 2.75                     | 0.49              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:86:HIS:C      | 5:F:88:ILE:N      | 2.65                     | 0.49              |
| 1:K:151:VAL:O     | 1:K:169:ALA:N     | 2.43                     | 0.49              |
| 1:K:20:TYR:CG     | 1:K:21:GLY:N      | 2.81                     | 0.49              |
| 1:L:37:GLY:O      | 1:L:38:ASN:C      | 2.51                     | 0.49              |
| 2:M:65:VAL:O      | 2:M:100:LEU:CD1   | 2.60                     | 0.49              |
| 2:M:1040:LEU:HD23 | 3:N:763:MET:HE1   | 1.94                     | 0.49              |
| 3:N:1107:VAL:HG21 | 3:N:1219:GLU:HB3  | 1.95                     | 0.49              |
| 3:N:1161:GLU:OE2  | 3:N:1164:ARG:HB2  | 2.11                     | 0.49              |
| 3:N:1311:LEU:HG   | 3:N:1312:LEU:N    | 2.28                     | 0.49              |
| 3:N:1397:LYS:O    | 3:N:1398:TRP:CD1  | 2.66                     | 0.49              |
| 3:N:1442:ASN:O    | 3:N:1446:VAL:HG23 | 2.12                     | 0.49              |
| 3:N:14:SER:O      | 3:N:17:LYS:HB3    | 2.13                     | 0.49              |
| 3:N:356:PRO:HB3   | 3:N:440:VAL:CG2   | 2.41                     | 0.49              |
| 3:N:59:ALA:C      | 3:N:61:GLY:N      | 2.65                     | 0.49              |
| 3:N:634:GLY:HA3   | 3:N:637:LEU:CD1   | 2.43                     | 0.49              |
| 3:N:676:MET:C     | 3:N:677:LEU:HD23  | 2.33                     | 0.49              |
| 3:N:756:GLN:O     | 3:N:759:ALA:HB3   | 2.12                     | 0.49              |
| 3:N:62:LYS:HE3    | 3:N:75:ARG:HH11   | 1.78                     | 0.49              |
| 3:N:859:ASP:O     | 3:N:862:ASP:HB2   | 2.13                     | 0.49              |
| 3:N:984:THR:HG22  | 3:N:987:GLU:CD    | 2.33                     | 0.49              |
| 3:N:696:HIS:CD2   | 4:O:48:MET:HG2    | 2.48                     | 0.49              |
| 1:A:152:PRO:O     | 1:A:155:LYS:HB3   | 2.13                     | 0.49              |
| 1:A:36:LEU:C      | 1:A:39:PRO:HD2    | 2.33                     | 0.49              |
| 1:B:32:PHE:O      | 1:B:33:GLY:C      | 2.50                     | 0.49              |
| 2:C:267:TYR:CB    | 2:C:272:ALA:H     | 2.26                     | 0.49              |
| 2:C:273:GLY:O     | 2:C:276:LYS:HB2   | 2.12                     | 0.49              |
| 2:C:32:ALA:O      | 2:C:35:PRO:HD2    | 2.13                     | 0.49              |
| 2:C:344:PHE:CE2   | 2:C:348:LEU:HD13  | 2.48                     | 0.49              |
| 2:C:493:ARG:HB2   | 2:C:494:TYR:CD1   | 2.48                     | 0.49              |
| 2:C:471:TYR:HB3   | 2:C:531:PHE:HD2   | 1.77                     | 0.49              |
| 2:C:92:ALA:C      | 2:C:117:HIS:HB3   | 2.32                     | 0.49              |
| 3:D:1020:LEU:O    | 3:D:1021:TYR:C    | 2.51                     | 0.49              |
| 3:D:1137:ARG:O    | 3:D:1138:ALA:C    | 2.51                     | 0.49              |
| 3:D:1291:SER:HA   | 3:D:1305:LEU:HD23 | 1.95                     | 0.49              |
| 2:C:1050:GLN:NE2  | 3:D:1469:GLY:O    | 2.40                     | 0.49              |
| 3:D:584:ASN:OD1   | 3:D:590:PRO:CD    | 2.55                     | 0.49              |
| 3:D:591:VAL:O     | 3:D:592:THR:C     | 2.50                     | 0.49              |
| 3:D:806:PHE:HZ    | 3:D:816:HIS:CE1   | 2.30                     | 0.49              |
| 3:D:811:GLU:HB3   | 3:D:815:ALA:CB    | 2.42                     | 0.49              |
| 3:D:87:ARG:CB     | 3:D:523:ASP:HB2   | 2.43                     | 0.49              |
| 2:C:971:LYS:HZ1   | 3:D:950:GLY:HA3   | 1.76                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:F:308:LEU:HD23  | 5:F:308:LEU:N    | 2.27                     | 0.49              |
| 5:F:418:LEU:N     | 5:F:418:LEU:HD12 | 2.11                     | 0.49              |
| 1:K:138:LEU:HD21  | 1:K:140:MET:CE   | 2.42                     | 0.49              |
| 1:L:56:VAL:N      | 1:L:165:ILE:O    | 2.44                     | 0.49              |
| 2:M:1017:THR:HB   | 2:M:1019:GLN:NE2 | 2.28                     | 0.49              |
| 2:M:237:ARG:O     | 2:M:240:THR:HB   | 2.12                     | 0.49              |
| 2:M:254:VAL:HB    | 2:M:258:TYR:OH   | 2.12                     | 0.49              |
| 2:M:37:GLU:OE2    | 2:M:71:TYR:O     | 2.29                     | 0.49              |
| 2:M:41:ASN:O      | 2:M:43:GLY:N     | 2.46                     | 0.49              |
| 2:M:589:ARG:HG2   | 2:M:596:TYR:OH   | 2.12                     | 0.49              |
| 2:M:610:ARG:HE    | 2:M:612:VAL:HG23 | 1.77                     | 0.49              |
| 2:M:874:LEU:HD13  | 3:N:783:ARG:HB3  | 1.94                     | 0.49              |
| 2:M:94:LEU:C      | 2:M:114:PHE:HA   | 2.33                     | 0.49              |
| 3:N:130:SER:HB3   | 3:N:132:TYR:HE1  | 1.72                     | 0.49              |
| 3:N:1406:ARG:CB   | 3:N:1412:LYS:HE2 | 2.40                     | 0.49              |
| 3:N:1489:GLN:HA   | 3:N:1492:LEU:CG  | 2.43                     | 0.49              |
| 3:N:565:ILE:HG23  | 3:N:566:ILE:N    | 2.13                     | 0.49              |
| 3:N:881:LEU:O     | 3:N:884:ARG:HB3  | 2.13                     | 0.49              |
| 3:N:972:LEU:HD23  | 3:N:972:LEU:H    | 1.78                     | 0.49              |
| 3:N:1497:GLU:HB2  | 4:O:88:GLU:OE2   | 2.12                     | 0.49              |
| 5:P:132:ARG:O     | 5:P:135:ILE:N    | 2.44                     | 0.49              |
| 5:P:145:PRO:HG3   | 5:P:150:THR:O    | 2.12                     | 0.49              |
| 5:P:296:GLY:C     | 5:P:299:TRP:HD1  | 2.17                     | 0.49              |
| 5:P:350:LEU:C     | 5:P:352:GLU:N    | 2.65                     | 0.49              |
| 1:A:208:LEU:O     | 1:A:209:GLU:C    | 2.51                     | 0.49              |
| 1:A:220:GLU:O     | 1:A:223:THR:HB   | 2.12                     | 0.49              |
| 1:B:112:ARG:CZ    | 1:B:125:PRO:HB2  | 2.42                     | 0.49              |
| 1:B:73:GLU:CB     | 1:B:78:ILE:HD11  | 2.43                     | 0.49              |
| 2:C:178:PRO:HA    | 2:C:181:VAL:O    | 2.13                     | 0.49              |
| 2:C:269:LEU:HA    | 2:C:288:ARG:CB   | 2.42                     | 0.49              |
| 2:C:726:ILE:HG13  | 2:C:728:HIS:HB3  | 1.94                     | 0.49              |
| 3:D:1346:ARG:HH11 | 3:D:1346:ARG:CG  | 2.25                     | 0.49              |
| 3:D:127:LEU:CD1   | 3:D:134:VAL:HG22 | 2.43                     | 0.49              |
| 3:D:1376:MET:CE   | 3:D:1421:LEU:HA  | 2.43                     | 0.49              |
| 3:D:1398:TRP:CB   | 3:D:1402:ALA:HB3 | 2.43                     | 0.49              |
| 3:D:234:GLU:O     | 3:D:236:TYR:N    | 2.41                     | 0.49              |
| 3:D:442:ASN:HD22  | 3:D:442:ASN:H    | 1.61                     | 0.49              |
| 3:D:857:ILE:HG13  | 3:D:858:VAL:HG23 | 1.94                     | 0.49              |
| 3:D:983:LEU:CD2   | 3:D:987:GLU:HB3  | 2.41                     | 0.49              |
| 4:E:92:ILE:HB     | 4:E:93:TYR:CD1   | 2.47                     | 0.49              |
| 5:F:161:GLN:O     | 5:F:165:SER:HB3  | 2.13                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:36:LEU:C      | 1:K:39:PRO:HD2   | 2.33                     | 0.49              |
| 2:M:1049:LEU:O    | 2:M:1053:LEU:HG  | 2.13                     | 0.49              |
| 2:M:208:ALA:O     | 2:M:212:GLY:HA3  | 2.12                     | 0.49              |
| 2:M:705:ILE:O     | 2:M:705:ILE:HG23 | 2.13                     | 0.49              |
| 2:M:916:GLU:O     | 2:M:919:ALA:HB3  | 2.12                     | 0.49              |
| 2:M:95:TYR:HA     | 2:M:113:VAL:O    | 2.13                     | 0.49              |
| 3:N:100:ALA:HB3   | 3:N:575:GLN:HE22 | 1.77                     | 0.49              |
| 3:N:1026:SER:C    | 3:N:1028:ALA:H   | 2.17                     | 0.49              |
| 3:N:1046:GLN:HB2  | 3:N:1052:THR:HA  | 1.93                     | 0.49              |
| 3:N:1048:PRO:CG   | 3:N:1075:HIS:HD2 | 2.22                     | 0.49              |
| 3:N:1341:PRO:HG2  | 3:N:1342:GLU:CD  | 2.30                     | 0.49              |
| 3:N:1394:VAL:HG11 | 3:N:1397:LYS:HE3 | 1.94                     | 0.49              |
| 3:N:1445:HIS:O    | 3:N:1446:VAL:C   | 2.49                     | 0.49              |
| 3:N:187:LYS:N     | 3:N:200:ASP:OD2  | 2.46                     | 0.49              |
| 3:N:322:VAL:HA    | 3:N:335:LEU:CD1  | 2.42                     | 0.49              |
| 3:N:421:LEU:HD11  | 3:N:429:SER:HB3  | 1.95                     | 0.49              |
| 3:N:441:ARG:O     | 3:N:442:ASN:C    | 2.51                     | 0.49              |
| 3:N:401:TYR:HB2   | 3:N:444:VAL:HG23 | 1.95                     | 0.49              |
| 3:N:521:PRO:C     | 3:N:525:ARG:NH1  | 2.66                     | 0.49              |
| 3:N:657:LEU:O     | 3:N:658:LEU:C    | 2.51                     | 0.49              |
| 3:N:806:PHE:CE2   | 3:N:812:ALA:HB3  | 2.47                     | 0.49              |
| 3:N:895:VAL:O     | 3:N:899:LEU:HG   | 2.12                     | 0.49              |
| 5:P:115:LYS:O     | 5:P:119:ILE:HG13 | 2.13                     | 0.49              |
| 1:A:57:TYR:CE1    | 1:A:163:ASN:HB2  | 2.46                     | 0.48              |
| 1:A:16:GLN:CD     | 1:B:235:ALA:HB1  | 2.33                     | 0.48              |
| 1:A:213:GLN:O     | 1:A:214:ALA:C    | 2.51                     | 0.48              |
| 2:C:20:GLU:C      | 2:C:23:VAL:HG22  | 2.33                     | 0.48              |
| 2:C:424:GLY:O     | 2:C:428:ARG:HG3  | 2.13                     | 0.48              |
| 2:C:499:ALA:HB2   | 2:C:533:ASP:O    | 2.13                     | 0.48              |
| 2:C:498:GLN:HB3   | 2:C:500:ASN:OD1  | 2.13                     | 0.48              |
| 2:C:48:PHE:CE1    | 2:C:71:TYR:HB3   | 2.48                     | 0.48              |
| 2:C:800:VAL:HG12  | 2:C:801:VAL:N    | 2.28                     | 0.48              |
| 2:C:833:LEU:HD12  | 2:C:837:ASP:OD2  | 2.13                     | 0.48              |
| 2:C:874:LEU:HB3   | 3:D:1029:ARG:HD3 | 1.95                     | 0.48              |
| 2:C:939:ARG:HD2   | 2:C:982:PRO:HD3  | 1.94                     | 0.48              |
| 3:D:1117:TYR:HD1  | 3:D:1118:ILE:O   | 1.96                     | 0.48              |
| 3:D:1466:VAL:O    | 3:D:1468:LEU:N   | 2.46                     | 0.48              |
| 3:D:226:PRO:HB2   | 3:D:231:VAL:HG21 | 1.94                     | 0.48              |
| 3:D:470:LEU:HB2   | 3:D:503:LEU:CD2  | 2.42                     | 0.48              |
| 3:D:783:ARG:CZ    | 3:D:1029:ARG:NH1 | 2.76                     | 0.48              |
| 3:D:827:ILE:CA    | 3:D:836:VAL:HB   | 2.38                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:E:86:GLN:O      | 4:E:90:GLU:HG3   | 2.13                     | 0.48              |
| 5:F:130:VAL:O     | 5:F:131:VAL:C    | 2.52                     | 0.48              |
| 1:K:100:LEU:HD23  | 1:K:101:LEU:N    | 2.23                     | 0.48              |
| 1:K:153:ALA:HA    | 1:K:156:HIS:CE1  | 2.48                     | 0.48              |
| 1:K:152:PRO:HA    | 1:K:168:ASP:OD1  | 2.13                     | 0.48              |
| 1:L:83:LYS:CE     | 1:L:168:ASP:HB2  | 2.43                     | 0.48              |
| 1:L:91:ASN:CB     | 1:L:94:LEU:HG    | 2.39                     | 0.48              |
| 2:M:176:VAL:HG12  | 2:M:181:VAL:O    | 2.12                     | 0.48              |
| 2:M:230:ARG:O     | 2:M:230:ARG:HG2  | 2.13                     | 0.48              |
| 2:M:498:GLN:CD    | 3:N:1068:LEU:HB2 | 2.33                     | 0.48              |
| 2:M:554:ASP:OD2   | 2:M:556:ASN:HB2  | 2.12                     | 0.48              |
| 3:N:1137:ARG:O    | 3:N:1138:ALA:C   | 2.49                     | 0.48              |
| 3:N:1161:GLU:CG   | 3:N:1164:ARG:HB2 | 2.39                     | 0.48              |
| 3:N:225:LEU:O     | 3:N:330:THR:HA   | 2.13                     | 0.48              |
| 3:N:22:SER:HB2    | 3:N:92:HIS:ND1   | 2.28                     | 0.48              |
| 3:N:317:VAL:HG23  | 3:N:338:GLU:O    | 2.13                     | 0.48              |
| 3:N:712:GLY:C     | 3:N:713:ILE:HG13 | 2.33                     | 0.48              |
| 3:N:967:ALA:HB2   | 3:N:999:THR:HG21 | 1.95                     | 0.48              |
| 3:N:98:PRO:CA     | 3:N:514:LEU:O    | 2.60                     | 0.48              |
| 4:O:29:GLN:O      | 4:O:31:LEU:N     | 2.45                     | 0.48              |
| 5:P:300:ASP:OD1   | 5:P:302:LYS:HG3  | 2.12                     | 0.48              |
| 1:A:101:LEU:HD13  | 1:A:113:ASP:O    | 2.13                     | 0.48              |
| 1:A:43:ILE:CG2    | 1:A:47:SER:HB2   | 2.42                     | 0.48              |
| 2:C:258:TYR:CD2   | 2:C:258:TYR:N    | 2.79                     | 0.48              |
| 2:C:313:LEU:C     | 2:C:315:ALA:N    | 2.65                     | 0.48              |
| 2:C:471:TYR:CD1   | 2:C:486:MET:HE2  | 2.48                     | 0.48              |
| 2:C:612:VAL:HA    | 2:C:622:GLU:HA   | 1.95                     | 0.48              |
| 3:D:1041:LEU:HD21 | 3:D:1043:GLY:HA2 | 1.95                     | 0.48              |
| 3:D:1098:LEU:HD12 | 3:D:1098:LEU:N   | 2.27                     | 0.48              |
| 3:D:1105:ILE:HD11 | 3:D:1374:GLN:CD  | 2.32                     | 0.48              |
| 3:D:1440:PHE:HE2  | 3:D:1463:LYS:HZ3 | 1.60                     | 0.48              |
| 3:D:1465:ASN:ND2  | 3:D:1471:LEU:O   | 2.42                     | 0.48              |
| 3:D:175:VAL:HG11  | 3:D:192:ALA:HB1  | 1.93                     | 0.48              |
| 3:D:223:LEU:O     | 3:D:332:TYR:CD1  | 2.66                     | 0.48              |
| 3:D:318:ARG:CZ    | 3:D:338:GLU:OE2  | 2.61                     | 0.48              |
| 3:D:438:ASP:C     | 3:D:439:LEU:HD23 | 2.34                     | 0.48              |
| 3:D:989:TYR:O     | 3:D:992:ILE:HB   | 2.13                     | 0.48              |
| 3:D:55:ASP:OD2    | 5:F:337:HIS:NE2  | 2.46                     | 0.48              |
| 1:L:10:VAL:O      | 1:L:10:VAL:HG23  | 2.12                     | 0.48              |
| 1:L:72:LYS:HD3    | 1:L:72:LYS:C     | 2.33                     | 0.48              |
| 2:M:1033:GLY:O    | 2:M:1036:GLU:HB2 | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:198:ARG:HH21  | 2:M:231:PRO:CD   | 2.24                     | 0.48              |
| 2:M:193:LEU:CD2   | 2:M:307:LEU:HD13 | 2.43                     | 0.48              |
| 2:M:385:PHE:CD1   | 2:M:385:PHE:C    | 2.84                     | 0.48              |
| 2:M:557:ARG:O     | 2:M:844:GLY:HA3  | 2.13                     | 0.48              |
| 2:M:712:ALA:HA    | 2:M:720:GLU:OE1  | 2.13                     | 0.48              |
| 2:M:690:ILE:HB    | 2:M:852:ILE:HG12 | 1.95                     | 0.48              |
| 2:M:914:ILE:H     | 2:M:914:ILE:HD12 | 1.75                     | 0.48              |
| 3:N:119:SER:HB3   | 3:N:123:LEU:N    | 2.23                     | 0.48              |
| 3:N:1379:VAL:HA   | 3:N:1420:LEU:HB2 | 1.95                     | 0.48              |
| 3:N:1415:VAL:HG23 | 3:N:1415:VAL:O   | 2.13                     | 0.48              |
| 3:N:259:VAL:HG21  | 3:N:292:VAL:CA   | 2.43                     | 0.48              |
| 3:N:355:VAL:CG1   | 3:N:356:PRO:HD2  | 2.43                     | 0.48              |
| 3:N:702:LEU:O     | 3:N:736:PHE:HZ   | 1.95                     | 0.48              |
| 3:N:844:ALA:HB1   | 3:N:867:ARG:NH1  | 2.28                     | 0.48              |
| 3:N:896:ALA:O     | 3:N:900:ILE:HG13 | 2.12                     | 0.48              |
| 3:N:573:MET:CE    | 5:P:211:ASP:OD1  | 2.61                     | 0.48              |
| 5:P:288:TYR:C     | 5:P:291:ILE:HG23 | 2.32                     | 0.48              |
| 5:P:76:SER:C      | 5:P:78:SER:N     | 2.65                     | 0.48              |
| 5:P:75:ILE:CG1    | 5:P:76:SER:H     | 2.10                     | 0.48              |
| 2:C:182:VAL:CG2   | 2:C:221:LEU:HA   | 2.43                     | 0.48              |
| 2:C:389:SER:HB3   | 2:C:392:SER:CB   | 2.44                     | 0.48              |
| 3:D:128:TYR:OH    | 3:D:575:GLN:CD   | 2.51                     | 0.48              |
| 3:D:1397:LYS:CB   | 3:D:1398:TRP:CZ3 | 2.93                     | 0.48              |
| 3:D:152:LEU:CG    | 3:D:153:LEU:N    | 2.77                     | 0.48              |
| 3:D:241:ILE:HD13  | 3:D:310:LEU:HD22 | 1.93                     | 0.48              |
| 3:D:324:ALA:CB    | 3:D:331:VAL:HG11 | 2.44                     | 0.48              |
| 3:D:355:VAL:HG23  | 3:D:367:ILE:HG23 | 1.93                     | 0.48              |
| 3:D:162:ARG:HA    | 3:D:449:SER:OG   | 2.13                     | 0.48              |
| 3:D:41:ARG:NH2    | 3:D:48:ARG:NH1   | 2.61                     | 0.48              |
| 3:D:522:PRO:N     | 3:D:525:ARG:HH12 | 2.12                     | 0.48              |
| 2:C:1095:LEU:HG   | 3:D:603:LEU:HD13 | 1.93                     | 0.48              |
| 3:D:662:GLU:N     | 3:D:667:ALA:HB3  | 2.28                     | 0.48              |
| 3:D:793:THR:HG21  | 3:D:906:GLN:CG   | 2.41                     | 0.48              |
| 5:F:120:THR:CG2   | 5:F:122:LEU:HG   | 2.43                     | 0.48              |
| 1:K:206:THR:HB    | 1:K:209:GLU:OE1  | 2.13                     | 0.48              |
| 1:L:5:LYS:HZ3     | 1:L:189:ARG:NE   | 2.12                     | 0.48              |
| 2:M:203:ASP:CA    | 2:M:228:ALA:HB1  | 2.43                     | 0.48              |
| 2:M:17:PRO:O      | 2:M:20:GLU:HB2   | 2.14                     | 0.48              |
| 2:M:212:GLY:HA3   | 2:M:218:VAL:CG1  | 2.42                     | 0.48              |
| 2:M:309:TYR:CZ    | 2:M:321:GLU:HG3  | 2.47                     | 0.48              |
| 2:M:380:ALA:CA    | 2:M:384:GLU:HG2  | 2.44                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:685:GLU:HB3   | 3:N:740:PHE:HD1  | 1.77                     | 0.48              |
| 2:M:685:GLU:C     | 2:M:687:ALA:H    | 2.16                     | 0.48              |
| 2:M:691:SER:C     | 2:M:693:GLU:N    | 2.63                     | 0.48              |
| 2:M:764:GLU:HB3   | 2:M:766:GLU:OE2  | 2.12                     | 0.48              |
| 2:M:769:PRO:HG2   | 3:N:65:ARG:NH1   | 2.28                     | 0.48              |
| 2:M:808:ARG:O     | 2:M:810:ASP:N    | 2.46                     | 0.48              |
| 2:M:946:ARG:HH11  | 2:M:984:GLU:CB   | 2.26                     | 0.48              |
| 3:N:1092:GLY:O    | 3:N:1096:ARG:N   | 2.35                     | 0.48              |
| 3:N:1208:ASP:HB3  | 3:N:1211:MET:O   | 2.13                     | 0.48              |
| 3:N:105:VAL:HG13  | 3:N:124:GLU:OE2  | 2.13                     | 0.48              |
| 3:N:1372:VAL:O    | 3:N:1373:ARG:C   | 2.51                     | 0.48              |
| 3:N:245:LEU:HA    | 3:N:309:GLY:N    | 2.04                     | 0.48              |
| 3:N:39:PRO:HB3    | 3:N:45:PHE:O     | 2.12                     | 0.48              |
| 3:N:502:PHE:O     | 3:N:503:LEU:C    | 2.51                     | 0.48              |
| 3:N:69:GLU:CD     | 3:N:71:LYS:HZ1   | 2.17                     | 0.48              |
| 3:N:757:ALA:O     | 3:N:758:GLU:C    | 2.51                     | 0.48              |
| 4:O:19:LEU:O      | 4:O:20:THR:C     | 2.51                     | 0.48              |
| 2:M:1015:LEU:CD1  | 5:P:335:ASP:HB2  | 2.42                     | 0.48              |
| 1:A:111:ALA:O     | 1:A:114:PHE:HD1  | 1.97                     | 0.48              |
| 2:C:250:ARG:O     | 2:C:252:LYS:N    | 2.47                     | 0.48              |
| 2:C:550:LEU:HD22  | 2:C:905:ILE:HD11 | 1.96                     | 0.48              |
| 2:C:589:ARG:HG2   | 2:C:596:TYR:CZ   | 2.48                     | 0.48              |
| 2:C:603:VAL:HG11  | 2:C:644:VAL:C    | 2.34                     | 0.48              |
| 2:C:809:GLY:N     | 2:C:813:VAL:HB   | 2.28                     | 0.48              |
| 2:C:958:THR:O     | 2:C:959:PRO:C    | 2.52                     | 0.48              |
| 3:D:1046:GLN:CB   | 3:D:1052:THR:HA  | 2.44                     | 0.48              |
| 3:D:1345:GLU:O    | 3:D:1346:ARG:C   | 2.52                     | 0.48              |
| 3:D:1381:VAL:HG11 | 3:D:1388:ARG:O   | 2.13                     | 0.48              |
| 3:D:135:LEU:HG    | 3:D:151:GLN:O    | 2.13                     | 0.48              |
| 3:D:266:GLU:OE1   | 3:D:314:PRO:HB3  | 2.14                     | 0.48              |
| 3:D:491:LYS:O     | 3:D:494:LYS:HB2  | 2.13                     | 0.48              |
| 3:D:630:VAL:HG12  | 3:D:631:ILE:N    | 2.27                     | 0.48              |
| 3:D:661:MET:HE1   | 3:D:677:LEU:HD11 | 1.93                     | 0.48              |
| 4:E:29:GLN:CG     | 4:E:30:LEU:N     | 2.76                     | 0.48              |
| 4:E:40:LEU:HD13   | 4:E:72:ARG:HH12  | 1.78                     | 0.48              |
| 5:F:125:ASP:CG    | 5:F:126:LEU:N    | 2.67                     | 0.48              |
| 1:K:124:ASN:O     | 1:K:127:LEU:HB3  | 2.13                     | 0.48              |
| 1:L:167:VAL:HG12  | 1:L:168:ASP:N    | 2.27                     | 0.48              |
| 1:L:235:ALA:HB3   | 1:L:236:PRO:CD   | 2.35                     | 0.48              |
| 2:M:1118:LYS:HG3  | 2:M:1119:ARG:N   | 2.28                     | 0.48              |
| 2:M:198:ARG:NH1   | 2:M:203:ASP:HB3  | 2.28                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:230:ARG:CG    | 2:M:233:GLU:HG2   | 2.42                     | 0.48              |
| 2:M:321:GLU:H     | 2:M:321:GLU:CD    | 2.15                     | 0.48              |
| 2:M:549:PHE:CE2   | 2:M:886:LEU:CB    | 2.96                     | 0.48              |
| 2:M:560:MET:HB3   | 2:M:564:MET:HE1   | 1.94                     | 0.48              |
| 3:N:1047:LYS:HG2  | 3:N:1053:PHE:CZ   | 2.47                     | 0.48              |
| 3:N:1108:ARG:HD2  | 3:N:1199:GLY:HA3  | 1.95                     | 0.48              |
| 3:N:1405:GLU:O    | 3:N:1410:GLU:C    | 2.52                     | 0.48              |
| 3:N:795:VAL:HA    | 3:N:861:GLN:O     | 2.13                     | 0.48              |
| 3:N:984:THR:CG2   | 3:N:987:GLU:H     | 2.26                     | 0.48              |
| 5:P:146:GLY:HA3   | 5:P:149:GLU:OE2   | 2.14                     | 0.48              |
| 5:P:157:GLU:N     | 5:P:157:GLU:CD    | 2.66                     | 0.48              |
| 5:P:361:LEU:CG    | 5:P:362:SER:H     | 2.25                     | 0.48              |
| 1:A:211:LEU:O     | 1:A:214:ALA:HB3   | 2.13                     | 0.48              |
| 1:B:55:SER:HA     | 1:B:167:VAL:HG23  | 1.95                     | 0.48              |
| 2:C:1067:TYR:CB   | 5:F:341:PRO:HB3   | 2.43                     | 0.48              |
| 2:C:112:GLU:HA    | 2:C:112:GLU:OE1   | 2.14                     | 0.48              |
| 2:C:234:ALA:HA    | 2:C:237:ARG:HD2   | 1.94                     | 0.48              |
| 2:C:292:ARG:HE    | 2:C:295:ASP:CB    | 2.27                     | 0.48              |
| 2:C:529:VAL:HG12  | 2:C:530:GLU:N     | 2.29                     | 0.48              |
| 2:C:742:VAL:CG1   | 2:C:743:VAL:N     | 2.77                     | 0.48              |
| 2:C:838:LYS:HE3   | 2:C:997:LEU:HB3   | 1.95                     | 0.48              |
| 3:D:1117:TYR:O    | 3:D:1193:THR:HG21 | 2.13                     | 0.48              |
| 3:D:1443:THR:HG23 | 10:D:1529:NE6:H24 | 1.96                     | 0.48              |
| 3:D:186:VAL:O     | 3:D:189:GLN:HB2   | 2.13                     | 0.48              |
| 3:D:225:LEU:HD11  | 3:D:242:LEU:CD1   | 2.40                     | 0.48              |
| 3:D:217:LYS:O     | 3:D:339:TRP:HD1   | 1.96                     | 0.48              |
| 3:D:406:ASP:CB    | 3:D:423:ASP:HA    | 2.42                     | 0.48              |
| 3:D:493:ARG:HG3   | 3:D:494:LYS:N     | 2.27                     | 0.48              |
| 3:D:622:ARG:HH11  | 3:D:622:ARG:HG2   | 1.77                     | 0.48              |
| 3:D:692:GLU:O     | 3:D:693:GLU:C     | 2.52                     | 0.48              |
| 3:D:692:GLU:O     | 3:D:695:ILE:HB    | 2.14                     | 0.48              |
| 3:D:756:GLN:HE22  | 3:D:760:ARG:HD2   | 1.78                     | 0.48              |
| 3:D:914:LEU:HD12  | 3:D:914:LEU:C     | 2.33                     | 0.48              |
| 3:D:926:LYS:O     | 3:D:929:ARG:HB2   | 2.13                     | 0.48              |
| 3:D:932:ASP:O     | 3:D:935:LYS:HE2   | 2.13                     | 0.48              |
| 5:F:75:ILE:C      | 5:F:77:THR:H      | 2.15                     | 0.48              |
| 1:K:73:GLU:CD     | 1:K:73:GLU:H      | 2.17                     | 0.48              |
| 2:M:1008:ARG:NH2  | 2:M:1012:PRO:O    | 2.47                     | 0.48              |
| 2:M:108:ILE:HB    | 2:M:368:THR:CG2   | 2.27                     | 0.48              |
| 2:M:343:GLN:HG2   | 2:M:385:PHE:CG    | 2.49                     | 0.48              |
| 2:M:909:ALA:O     | 2:M:910:LYS:HD2   | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:916:GLU:OE1   | 2:M:916:GLU:C     | 2.52                     | 0.48              |
| 2:M:916:GLU:O     | 2:M:919:ALA:N     | 2.46                     | 0.48              |
| 2:M:944:LEU:HD11  | 2:M:963:LEU:HD21  | 1.96                     | 0.48              |
| 1:K:38:ASN:HB2    | 2:M:980:GLY:HA3   | 1.95                     | 0.48              |
| 3:N:1359:GLN:HG3  | 3:N:1359:GLN:O    | 2.12                     | 0.48              |
| 3:N:573:MET:HE3   | 5:P:210:LEU:HB2   | 1.96                     | 0.48              |
| 3:N:631:ILE:HG12  | 3:N:743:ASP:O     | 2.13                     | 0.48              |
| 3:N:673:ALA:C     | 3:N:676:MET:HB3   | 2.34                     | 0.48              |
| 3:N:703:ASN:HD22  | 3:N:704:ARG:H     | 1.60                     | 0.48              |
| 4:O:46:PRO:HG2    | 4:O:63:TRP:CD1    | 2.49                     | 0.48              |
| 5:P:367:MET:O     | 5:P:370:LYS:CG    | 2.61                     | 0.48              |
| 1:A:167:VAL:CG1   | 1:A:168:ASP:N     | 2.77                     | 0.48              |
| 1:B:151:VAL:O     | 1:B:169:ALA:N     | 2.47                     | 0.48              |
| 1:B:68:ILE:HD12   | 1:B:71:VAL:CB     | 2.42                     | 0.48              |
| 2:C:157:ARG:NH1   | 2:C:314:THR:HA    | 2.28                     | 0.48              |
| 2:C:230:ARG:HH11  | 2:C:230:ARG:CG    | 2.24                     | 0.48              |
| 2:C:854:PRO:O     | 2:C:857:ASP:OD2   | 2.31                     | 0.48              |
| 2:C:971:LYS:HZ2   | 3:D:950:GLY:HA3   | 1.78                     | 0.48              |
| 3:D:1336:LEU:HD12 | 3:D:1340:GLY:C    | 2.32                     | 0.48              |
| 3:D:1404:ASN:OD1  | 3:D:1409:ALA:HB2  | 2.13                     | 0.48              |
| 3:D:1458:GLU:O    | 3:D:1459:LEU:HD23 | 2.14                     | 0.48              |
| 3:D:208:PRO:O     | 3:D:209:ARG:HG3   | 2.13                     | 0.48              |
| 3:D:234:GLU:C     | 3:D:236:TYR:N     | 2.66                     | 0.48              |
| 3:D:285:PRO:O     | 3:D:286:VAL:C     | 2.52                     | 0.48              |
| 3:D:408:GLU:OE2   | 3:D:422:ALA:CB    | 2.62                     | 0.48              |
| 3:D:45:PHE:HB3    | 3:D:86:ARG:NH2    | 2.28                     | 0.48              |
| 3:D:475:LYS:HA    | 3:D:478:LEU:HB2   | 1.95                     | 0.48              |
| 3:D:571:LYS:O     | 3:D:574:LEU:HB3   | 2.13                     | 0.48              |
| 3:D:69:GLU:CG     | 3:D:70:GLY:H      | 2.27                     | 0.48              |
| 1:B:176:ARG:HD3   | 3:D:884:ARG:NH2   | 2.28                     | 0.48              |
| 3:D:564:GLU:HA    | 5:F:140:ARG:NH1   | 2.28                     | 0.48              |
| 5:F:295:MET:HG3   | 5:F:299:TRP:CE2   | 2.49                     | 0.48              |
| 5:F:92:PRO:C      | 5:F:94:LEU:H      | 2.16                     | 0.48              |
| 1:K:99:LEU:HB3    | 1:K:114:PHE:CD2   | 2.47                     | 0.48              |
| 1:K:162:ILE:HG13  | 1:K:163:ASN:N     | 2.27                     | 0.48              |
| 1:L:34:VAL:O      | 1:L:36:LEU:N      | 2.46                     | 0.48              |
| 1:L:80:LEU:HB3    | 3:N:844:ALA:CB    | 2.40                     | 0.48              |
| 2:M:154:ARG:HG2   | 2:M:156:GLY:H     | 1.78                     | 0.48              |
| 2:M:176:VAL:HG12  | 2:M:182:VAL:HA    | 1.95                     | 0.48              |
| 2:M:751:PRO:CB    | 2:M:794:PRO:HA    | 2.29                     | 0.48              |
| 3:N:1068:LEU:O    | 3:N:1069:GLU:C    | 2.52                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1231:GLU:HB3  | 3:N:1232:PRO:HD3  | 1.95                     | 0.48              |
| 3:N:357:GLU:O     | 3:N:358:GLY:C     | 2.52                     | 0.48              |
| 3:N:522:PRO:N     | 3:N:525:ARG:NH1   | 2.60                     | 0.48              |
| 3:N:632:VAL:O     | 3:N:727:GLN:HA    | 2.14                     | 0.48              |
| 3:N:799:LYS:N     | 3:N:829:VAL:HG12  | 2.28                     | 0.48              |
| 3:N:806:PHE:H     | 3:N:809:PRO:HG2   | 1.79                     | 0.48              |
| 3:N:860:LEU:O     | 3:N:877:PRO:HD2   | 2.13                     | 0.48              |
| 5:P:103:ALA:HB1   | 5:P:229:TYR:HB3   | 1.95                     | 0.48              |
| 5:P:202:TYR:CD2   | 5:P:205:ARG:NH1   | 2.82                     | 0.48              |
| 1:A:167:VAL:HG12  | 1:A:168:ASP:H     | 1.75                     | 0.48              |
| 1:A:5:LYS:HZ3     | 1:A:192:LEU:HD22  | 1.77                     | 0.48              |
| 1:A:41:ARG:O      | 1:A:45:LEU:HG     | 2.14                     | 0.48              |
| 1:B:216:GLU:O     | 1:B:217:ILE:C     | 2.52                     | 0.48              |
| 1:B:239:ALA:C     | 1:B:241:GLU:N     | 2.67                     | 0.48              |
| 2:C:1000:MET:HB3  | 2:C:1002:GLU:CG   | 2.34                     | 0.48              |
| 2:C:65:VAL:CG2    | 2:C:101:ILE:HB    | 2.43                     | 0.48              |
| 2:C:1075:ASP:OD1  | 2:C:1076:VAL:N    | 2.41                     | 0.48              |
| 2:C:157:ARG:HD3   | 2:C:158:TYR:CE1   | 2.49                     | 0.48              |
| 2:C:446:GLY:O     | 2:C:448:ASN:N     | 2.46                     | 0.48              |
| 2:C:409:ARG:HA    | 2:C:453:THR:O     | 2.13                     | 0.48              |
| 2:C:753:ASP:O     | 2:C:791:ARG:HA    | 2.13                     | 0.48              |
| 2:C:930:LYS:C     | 2:C:932:GLU:N     | 2.66                     | 0.48              |
| 3:D:1098:LEU:O    | 3:D:1102:THR:N    | 2.46                     | 0.48              |
| 3:D:1178:ALA:HB2  | 3:D:1183:ILE:HG23 | 1.95                     | 0.48              |
| 3:D:1216:SER:HB2  | 4:E:16:LYS:H      | 1.76                     | 0.48              |
| 3:D:1335:LEU:HD11 | 3:D:1343:ALA:HB1  | 1.95                     | 0.48              |
| 3:D:1353:GLN:HB3  | 3:D:1357:ARG:CZ   | 2.43                     | 0.48              |
| 3:D:14:SER:C      | 3:D:16:GLU:N      | 2.65                     | 0.48              |
| 3:D:543:LEU:O     | 3:D:546:ARG:CG    | 2.50                     | 0.48              |
| 3:D:769:LEU:O     | 3:D:778:LEU:N     | 2.45                     | 0.48              |
| 3:D:792:ILE:O     | 3:D:878:GLY:HA3   | 2.13                     | 0.48              |
| 3:D:55:ASP:HA     | 3:D:83:SER:N      | 2.29                     | 0.48              |
| 3:D:96:ALA:O      | 5:F:144:ILE:HD11  | 2.14                     | 0.48              |
| 5:F:361:LEU:CG    | 5:F:362:SER:N     | 2.77                     | 0.48              |
| 2:M:174:LEU:CD2   | 2:M:184:MET:HG2   | 2.43                     | 0.48              |
| 2:M:304:LEU:CB    | 2:M:305:PRO:CD    | 2.85                     | 0.48              |
| 2:M:100:LEU:CD2   | 2:M:368:THR:HG23  | 2.41                     | 0.48              |
| 2:M:41:ASN:HB2    | 2:M:46:ALA:CA     | 2.43                     | 0.48              |
| 2:M:610:ARG:HD2   | 2:M:622:GLU:CG    | 2.44                     | 0.48              |
| 2:M:614:ARG:HA    | 2:M:619:ARG:O     | 2.14                     | 0.48              |
| 2:M:881:ASN:ND2   | 2:M:881:ASN:H     | 1.97                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:979:THR:C     | 2:M:981:GLU:N     | 2.67                     | 0.48              |
| 3:N:113:GLY:C     | 3:N:115:LEU:N     | 2.67                     | 0.48              |
| 3:N:1233:GLY:O    | 3:N:1235:GLN:N    | 2.47                     | 0.48              |
| 3:N:1277:ILE:CG2  | 3:N:1278:ASP:N    | 2.75                     | 0.48              |
| 3:N:1290:LEU:O    | 3:N:1305:LEU:HD23 | 2.13                     | 0.48              |
| 3:N:1313:VAL:HG22 | 3:N:1314:LYS:H    | 1.78                     | 0.48              |
| 3:N:173:PRO:CA    | 3:N:209:ARG:NH1   | 2.76                     | 0.48              |
| 3:N:458:ALA:HB1   | 3:N:513:ILE:CD1   | 2.38                     | 0.48              |
| 3:N:477:LEU:C     | 3:N:479:GLU:N     | 2.67                     | 0.48              |
| 3:N:493:ARG:HG3   | 3:N:494:LYS:N     | 2.29                     | 0.48              |
| 3:N:761:ILE:CD1   | 4:O:20:THR:HA     | 2.43                     | 0.48              |
| 3:N:811:GLU:HB3   | 3:N:815:ALA:HB3   | 1.94                     | 0.48              |
| 3:N:767:HIS:HA    | 3:N:924:MET:HE2   | 1.96                     | 0.48              |
| 3:N:997:THR:O     | 3:N:1000:THR:HB   | 2.14                     | 0.48              |
| 5:P:117:SER:O     | 5:P:121:GLY:N     | 2.45                     | 0.48              |
| 5:P:287:THR:HG23  | 5:P:289:GLU:OE1   | 2.14                     | 0.48              |
| 5:P:288:TYR:HB2   | 5:P:289:GLU:OE2   | 2.14                     | 0.48              |
| 5:P:321:ILE:CG1   | 5:P:332:PHE:HE1   | 2.24                     | 0.48              |
| 5:P:418:LEU:O     | 5:P:421:PHE:HA    | 2.13                     | 0.48              |
| 1:B:235:ALA:O     | 1:B:237:GLU:N     | 2.46                     | 0.48              |
| 2:C:1033:GLY:O    | 2:C:1037:VAL:HG23 | 2.13                     | 0.48              |
| 2:C:198:ARG:HE    | 2:C:231:PRO:HD3   | 1.77                     | 0.48              |
| 2:C:317:VAL:H     | 2:C:318:PRO:HD3   | 1.74                     | 0.48              |
| 2:C:413:LEU:HA    | 2:C:419:THR:HG23  | 1.94                     | 0.48              |
| 2:C:603:VAL:HG21  | 2:C:644:VAL:O     | 2.14                     | 0.48              |
| 2:C:625:LEU:CD1   | 2:C:639:GLN:HB2   | 2.31                     | 0.48              |
| 2:C:648:ARG:O     | 2:C:649:VAL:HG23  | 2.14                     | 0.48              |
| 2:C:832:LYS:HG2   | 2:C:833:LEU:H     | 1.79                     | 0.48              |
| 2:C:926:PHE:O     | 2:C:927:GLY:C     | 2.52                     | 0.48              |
| 2:C:923:GLU:O     | 2:C:927:GLY:N     | 2.46                     | 0.48              |
| 3:D:1059:SER:HB2  | 3:D:1065:LEU:CD2  | 2.44                     | 0.48              |
| 3:D:1378:TYR:O    | 3:D:1420:LEU:HB2  | 2.13                     | 0.48              |
| 3:D:1481:VAL:O    | 3:D:1483:PHE:N    | 2.47                     | 0.48              |
| 3:D:181:ASP:C     | 3:D:183:GLU:N     | 2.61                     | 0.48              |
| 3:D:355:VAL:CG1   | 3:D:359:ALA:HB3   | 2.44                     | 0.48              |
| 3:D:352:ASN:N     | 3:D:369:ALA:O     | 2.44                     | 0.48              |
| 3:D:630:VAL:HG22  | 3:D:744:GLN:HG3   | 1.96                     | 0.48              |
| 1:B:63:HIS:CD2    | 3:D:813:LEU:HD13  | 2.48                     | 0.48              |
| 3:D:828:LYS:O     | 3:D:828:LYS:HE2   | 2.13                     | 0.48              |
| 3:D:906:GLN:NE2   | 3:D:906:GLN:HA    | 2.28                     | 0.48              |
| 3:D:969:ARG:CG    | 3:D:970:LYS:N     | 2.76                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:154:GLU:HG2   | 3:N:840:LYS:HE3  | 1.95                     | 0.48              |
| 2:M:1060:ILE:O    | 2:M:1062:GLY:N   | 2.47                     | 0.48              |
| 2:M:218:VAL:HG11  | 2:M:222:MET:HE2  | 1.96                     | 0.48              |
| 2:M:38:LYS:CG     | 2:M:39:ARG:H     | 2.12                     | 0.48              |
| 2:M:432:ARG:CG    | 2:M:433:THR:N    | 2.77                     | 0.48              |
| 2:M:439:CYS:SG    | 2:M:441:VAL:CG1  | 3.02                     | 0.48              |
| 2:M:455:LEU:HD11  | 2:M:459:ALA:CB   | 2.43                     | 0.48              |
| 2:M:462:ASP:O     | 2:M:464:LEU:N    | 2.47                     | 0.48              |
| 2:M:564:MET:HA    | 2:M:567:GLN:NE2  | 2.29                     | 0.48              |
| 2:M:757:GLY:HA2   | 2:M:789:SER:CB   | 2.43                     | 0.48              |
| 2:M:75:GLU:O      | 2:M:77:PRO:CD    | 2.61                     | 0.48              |
| 2:M:672:VAL:HG23  | 2:M:868:ASP:HB2  | 1.96                     | 0.48              |
| 2:M:930:LYS:C     | 2:M:932:GLU:N    | 2.67                     | 0.48              |
| 3:N:1167:SER:HB3  | 3:N:1170:ASP:OD1 | 2.14                     | 0.48              |
| 3:N:169:TYR:O     | 3:N:392:SER:HA   | 2.14                     | 0.48              |
| 3:N:27:GLU:O      | 3:N:28:LYS:HD3   | 2.13                     | 0.48              |
| 3:N:433:GLY:CA    | 3:N:447:VAL:O    | 2.56                     | 0.48              |
| 3:N:540:LEU:O     | 3:N:543:LEU:HB2  | 2.14                     | 0.48              |
| 3:N:548:ILE:O     | 3:N:549:ASN:C    | 2.52                     | 0.48              |
| 3:N:557:LEU:HG    | 3:N:557:LEU:H    | 1.33                     | 0.48              |
| 3:N:790:TYR:HA    | 3:N:793:THR:OG1  | 2.13                     | 0.48              |
| 5:P:287:THR:HG23  | 5:P:290:GLU:OE1  | 2.13                     | 0.48              |
| 1:B:151:VAL:HG21  | 1:B:171:PHE:HE1  | 1.79                     | 0.48              |
| 2:C:144:PRO:HB3   | 2:C:163:ILE:O    | 2.13                     | 0.48              |
| 2:C:198:ARG:HE    | 2:C:231:PRO:HG3  | 1.78                     | 0.48              |
| 2:C:436:GLY:O     | 2:C:459:ALA:HB2  | 2.13                     | 0.48              |
| 2:C:644:VAL:O     | 2:C:647:GLN:CB   | 2.62                     | 0.48              |
| 2:C:773:LEU:O     | 2:C:776:SER:OG   | 2.26                     | 0.48              |
| 2:C:848:VAL:HG12  | 2:C:849:VAL:N    | 2.27                     | 0.48              |
| 2:C:914:ILE:O     | 2:C:916:GLU:N    | 2.46                     | 0.48              |
| 3:D:1078:ARG:HG3  | 3:D:1078:ARG:NH1 | 2.29                     | 0.48              |
| 3:D:1128:VAL:HG21 | 3:D:1131:SER:CB  | 2.34                     | 0.48              |
| 3:D:1311:LEU:HD12 | 3:D:1312:LEU:N   | 2.23                     | 0.48              |
| 3:D:1472:ILE:CD1  | 3:D:1473:PRO:HD2 | 2.38                     | 0.48              |
| 3:D:1106:VAL:HG11 | 3:D:1474:ALA:HB2 | 1.95                     | 0.48              |
| 3:D:318:ARG:CG    | 3:D:319:ALA:N    | 2.76                     | 0.48              |
| 3:D:564:GLU:HA    | 3:D:567:ILE:HG13 | 1.95                     | 0.48              |
| 3:D:965:GLU:O     | 3:D:966:GLU:C    | 2.50                     | 0.48              |
| 4:E:40:LEU:HD21   | 4:E:44:GLU:HB3   | 1.96                     | 0.48              |
| 5:F:115:LYS:HB3   | 5:F:119:ILE:CD1  | 2.44                     | 0.48              |
| 5:F:291:ILE:HD11  | 5:F:295:MET:HB2  | 1.96                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:F:362:SER:O     | 5:F:366:ALA:N      | 2.44                     | 0.48              |
| 1:K:103:ALA:C     | 1:K:104:GLU:HG3    | 2.34                     | 0.48              |
| 1:K:107:LYS:CE    | 1:K:108:GLU:O      | 2.62                     | 0.48              |
| 1:K:138:LEU:HD12  | 1:K:139:ASN:N      | 2.26                     | 0.48              |
| 1:K:186:LEU:C     | 1:K:188:GLN:N      | 2.59                     | 0.48              |
| 1:K:176:ARG:HB3   | 1:K:200:TRP:CD1    | 2.48                     | 0.48              |
| 1:K:1:MET:CA      | 1:K:6:LEU:HD22     | 2.43                     | 0.48              |
| 1:L:128:HIS:CE1   | 1:L:131:THR:HG23   | 2.49                     | 0.48              |
| 2:M:1023:GLY:N    | 2:M:1026:GLN:O     | 2.46                     | 0.48              |
| 2:M:1083:GLU:O    | 2:M:1084:SER:C     | 2.52                     | 0.48              |
| 2:M:230:ARG:HD3   | 2:M:230:ARG:H      | 1.76                     | 0.48              |
| 2:M:575:GLN:HE21  | 2:M:670:GLN:CB     | 2.24                     | 0.48              |
| 2:M:604:ALA:HB3   | 2:M:612:VAL:C      | 2.33                     | 0.48              |
| 3:N:1223:ILE:HD11 | 10:N:1528:NE6:H14B | 1.96                     | 0.48              |
| 3:N:1223:ILE:O    | 3:N:1224:VAL:C     | 2.51                     | 0.48              |
| 3:N:1257:PRO:HA   | 3:N:1260:ILE:HD12  | 1.96                     | 0.48              |
| 3:N:131:LYS:HB3   | 3:N:131:LYS:NZ     | 2.28                     | 0.48              |
| 3:N:136:ASP:HB2   | 3:N:137:PRO:CD     | 2.35                     | 0.48              |
| 3:N:1488:ASP:OD1  | 3:N:1491:THR:HB    | 2.14                     | 0.48              |
| 3:N:259:VAL:O     | 3:N:260:GLU:CG     | 2.62                     | 0.48              |
| 3:N:41:ARG:HH21   | 3:N:48:ARG:CZ      | 2.27                     | 0.48              |
| 2:M:1101:THR:CB   | 3:N:5:VAL:HG21     | 2.28                     | 0.48              |
| 3:N:630:VAL:HG22  | 3:N:744:GLN:HG2    | 1.95                     | 0.48              |
| 3:N:951:ILE:HD11  | 3:N:1062:ARG:HG3   | 1.95                     | 0.48              |
| 3:N:1481:VAL:HG11 | 4:O:18:ARG:HA      | 1.96                     | 0.48              |
| 1:A:29:GLU:HB3    | 1:A:32:PHE:CD1     | 2.49                     | 0.48              |
| 2:C:191:PHE:CZ    | 2:C:196:LEU:HD21   | 2.49                     | 0.48              |
| 2:C:178:PRO:C     | 2:C:220:GLY:HA2    | 2.25                     | 0.48              |
| 2:C:483:VAL:CG2   | 2:C:484:VAL:N      | 2.77                     | 0.48              |
| 2:C:542:VAL:O     | 2:C:545:ASN:HB2    | 2.14                     | 0.48              |
| 2:C:599:GLU:HG3   | 2:C:600:ASP:N      | 2.28                     | 0.48              |
| 2:C:673:LEU:HA    | 2:C:673:LEU:HD23   | 1.73                     | 0.48              |
| 2:C:698:ASP:HA    | 2:C:832:LYS:HE3    | 1.96                     | 0.48              |
| 2:C:722:ILE:O     | 2:C:722:ILE:HG13   | 2.13                     | 0.48              |
| 3:D:1066:THR:HG22 | 3:D:1068:LEU:N     | 2.28                     | 0.48              |
| 3:D:1106:VAL:O    | 3:D:1108:ARG:HG3   | 2.14                     | 0.48              |
| 3:D:110:SER:O     | 3:D:111:LYS:C      | 2.52                     | 0.48              |
| 3:D:1353:GLN:HB3  | 3:D:1357:ARG:NE    | 2.29                     | 0.48              |
| 3:D:1380:GLU:HA   | 3:D:1392:GLY:HA2   | 1.95                     | 0.48              |
| 3:D:178:LEU:HG    | 3:D:181:ASP:CG     | 2.34                     | 0.48              |
| 3:D:191:LEU:HD23  | 3:D:195:VAL:HG12   | 1.96                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:288:MET:HE1   | 3:D:307:ALA:HB2   | 1.95                     | 0.48              |
| 3:D:368:VAL:O     | 3:D:377:VAL:HB    | 2.14                     | 0.48              |
| 3:D:664:LYS:O     | 3:D:665:GLY:C     | 2.53                     | 0.48              |
| 4:E:24:ALA:O      | 4:E:27:ALA:HB3    | 2.14                     | 0.48              |
| 4:E:33:HIS:HB2    | 4:E:37:ASN:OD1    | 2.14                     | 0.48              |
| 5:F:399:GLN:O     | 5:F:402:ASN:HB2   | 2.14                     | 0.48              |
| 1:K:41:ARG:CG     | 1:K:45:LEU:HD11   | 2.41                     | 0.48              |
| 2:M:1048:THR:O    | 2:M:1051:GLU:HG3  | 2.14                     | 0.48              |
| 2:M:340:MET:C     | 2:M:340:MET:SD    | 2.92                     | 0.48              |
| 2:M:643:VAL:HG23  | 2:M:647:GLN:OE1   | 2.13                     | 0.48              |
| 2:M:68:PHE:HZ     | 2:M:71:TYR:N      | 2.11                     | 0.48              |
| 3:N:1118:ILE:HG23 | 3:N:1193:THR:HG23 | 1.96                     | 0.48              |
| 3:N:1364:HIS:CE1  | 3:N:1366:LYS:HG3  | 2.49                     | 0.48              |
| 3:N:361:VAL:HG11  | 3:N:367:ILE:HD11  | 1.96                     | 0.48              |
| 3:N:414:ARG:C     | 3:N:415:VAL:HG13  | 2.35                     | 0.48              |
| 3:N:565:ILE:HD11  | 5:P:87:GLU:OE2    | 2.13                     | 0.48              |
| 3:N:570:GLU:CA    | 5:P:214:GLN:HE21  | 2.27                     | 0.48              |
| 3:N:685:ASP:O     | 3:N:686:GLU:C     | 2.52                     | 0.48              |
| 3:N:884:ARG:O     | 3:N:888:GLU:HG2   | 2.13                     | 0.48              |
| 4:O:18:ARG:O      | 4:O:19:LEU:C      | 2.51                     | 0.48              |
| 5:P:111:GLU:HA    | 5:P:114:LYS:HG3   | 1.96                     | 0.48              |
| 5:P:235:PHE:O     | 5:P:236:SER:C     | 2.52                     | 0.48              |
| 5:P:361:LEU:HG    | 5:P:366:ALA:HB2   | 1.94                     | 0.48              |
| 1:B:186:LEU:HG    | 1:B:188:GLN:OE1   | 2.14                     | 0.47              |
| 1:B:97:VAL:CG1    | 1:B:98:THR:N      | 2.74                     | 0.47              |
| 2:C:257:VAL:CA    | 2:C:261:ILE:HD12  | 2.28                     | 0.47              |
| 2:C:430:VAL:HB    | 3:D:1078:ARG:NH1  | 2.29                     | 0.47              |
| 2:C:428:ARG:NH2   | 2:C:447:ALA:O     | 2.44                     | 0.47              |
| 2:C:463:GLU:CD    | 2:C:463:GLU:N     | 2.67                     | 0.47              |
| 2:C:572:ILE:HG13  | 2:C:573:ARG:HG3   | 1.96                     | 0.47              |
| 2:C:595:LEU:O     | 2:C:655:LEU:N     | 2.47                     | 0.47              |
| 3:D:1078:ARG:O    | 3:D:1079:LYS:C    | 2.53                     | 0.47              |
| 3:D:1085:ALA:CA   | 3:D:1088:THR:HG22 | 2.43                     | 0.47              |
| 3:D:1287:GLU:N    | 3:D:1288:GLU:OE1  | 2.47                     | 0.47              |
| 3:D:168:THR:HB    | 3:D:206:ARG:NH1   | 2.29                     | 0.47              |
| 3:D:270:LEU:HD12  | 3:D:271:VAL:N     | 2.28                     | 0.47              |
| 3:D:313:MET:SD    | 3:D:314:PRO:CD    | 2.95                     | 0.47              |
| 3:D:225:LEU:O     | 3:D:331:VAL:N     | 2.47                     | 0.47              |
| 3:D:36:THR:HB     | 3:D:38:LYS:CG     | 2.38                     | 0.47              |
| 3:D:65:ARG:HD2    | 3:D:66:GLN:H      | 1.79                     | 0.47              |
| 3:D:760:ARG:NH1   | 4:E:59:ASN:OD1    | 2.40                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:F:132:ARG:O     | 5:F:135:ILE:N    | 2.47                     | 0.47              |
| 5:F:261:PRO:CD    | 5:F:264:MET:HG3  | 2.39                     | 0.47              |
| 1:L:106:PRO:CA    | 1:L:133:GLU:HA   | 2.36                     | 0.47              |
| 2:M:1076:VAL:HG12 | 2:M:1077:PRO:N   | 2.29                     | 0.47              |
| 2:M:252:LYS:O     | 2:M:255:ALA:HB3  | 2.14                     | 0.47              |
| 2:M:252:LYS:HD3   | 2:M:298:PHE:HE1  | 1.79                     | 0.47              |
| 2:M:685:GLU:HB3   | 3:N:740:PHE:CE1  | 2.48                     | 0.47              |
| 2:M:430:VAL:HG12  | 3:N:1075:HIS:HA  | 1.95                     | 0.47              |
| 3:N:1366:LYS:O    | 3:N:1369:GLU:N   | 2.47                     | 0.47              |
| 3:N:1378:TYR:HB2  | 3:N:1422:MET:HE3 | 1.96                     | 0.47              |
| 3:N:202:VAL:O     | 3:N:395:VAL:HA   | 2.14                     | 0.47              |
| 3:N:252:ARG:HG3   | 3:N:300:LYS:O    | 2.14                     | 0.47              |
| 3:N:361:VAL:HG13  | 3:N:365:ASP:CB   | 2.21                     | 0.47              |
| 3:N:368:VAL:N     | 3:N:377:VAL:HB   | 2.29                     | 0.47              |
| 3:N:409:VAL:HG12  | 3:N:410:SER:N    | 2.28                     | 0.47              |
| 3:N:622:ARG:HG2   | 3:N:622:ARG:NH1  | 2.28                     | 0.47              |
| 3:N:676:MET:HG3   | 3:N:677:LEU:HD21 | 1.95                     | 0.47              |
| 3:N:69:GLU:CG     | 3:N:71:LYS:HZ3   | 2.27                     | 0.47              |
| 3:N:703:ASN:ND2   | 3:N:704:ARG:N    | 2.62                     | 0.47              |
| 3:N:984:THR:HG22  | 3:N:987:GLU:HG3  | 1.93                     | 0.47              |
| 5:P:104:ARG:HG3   | 5:P:105:LYS:N    | 2.29                     | 0.47              |
| 5:P:288:TYR:O     | 5:P:292:ALA:N    | 2.33                     | 0.47              |
| 5:P:370:LYS:HA    | 5:P:374:GLY:N    | 2.28                     | 0.47              |
| 5:P:409:LYS:HG3   | 5:P:410:TYR:H    | 1.78                     | 0.47              |
| 5:P:77:THR:C      | 5:P:79:ASP:N     | 2.66                     | 0.47              |
| 1:A:128:HIS:HE1   | 1:A:131:THR:HG23 | 1.77                     | 0.47              |
| 1:A:153:ALA:HA    | 1:A:156:HIS:CE1  | 2.48                     | 0.47              |
| 1:A:41:ARG:NH1    | 1:A:177:VAL:O    | 2.46                     | 0.47              |
| 1:A:220:GLU:O     | 1:A:223:THR:CB   | 2.62                     | 0.47              |
| 1:A:1:MET:N       | 1:A:6:LEU:HD13   | 2.29                     | 0.47              |
| 1:B:111:ALA:HA    | 1:B:129:ILE:HD11 | 1.95                     | 0.47              |
| 2:C:198:ARG:O     | 2:C:201:GLY:N    | 2.46                     | 0.47              |
| 2:C:419:THR:O     | 2:C:420:ARG:HG3  | 2.15                     | 0.47              |
| 2:C:708:TYR:N     | 2:C:708:TYR:CD1  | 2.82                     | 0.47              |
| 2:C:874:LEU:O     | 3:D:1029:ARG:HD3 | 2.14                     | 0.47              |
| 3:D:1066:THR:CB   | 3:D:1069:GLU:HG3 | 2.44                     | 0.47              |
| 3:D:1094:LEU:CD2  | 3:D:1230:GLY:HA2 | 2.37                     | 0.47              |
| 3:D:118:LEU:CA    | 3:D:123:LEU:HD12 | 2.33                     | 0.47              |
| 3:D:1286:THR:HB   | 3:D:1289:LYS:O   | 2.13                     | 0.47              |
| 3:D:473:LEU:O     | 3:D:476:GLU:HB3  | 2.13                     | 0.47              |
| 3:D:591:VAL:HG12  | 3:D:599:PRO:CA   | 2.43                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:614:PHE:CD2   | 3:D:617:ASN:ND2   | 2.82                     | 0.47              |
| 5:F:156:VAL:HG23  | 5:F:157:GLU:N     | 2.25                     | 0.47              |
| 5:F:91:VAL:C      | 5:F:93:LEU:H      | 2.18                     | 0.47              |
| 1:K:205:VAL:HG12  | 1:K:206:THR:N     | 2.29                     | 0.47              |
| 1:L:105:GLY:O     | 1:L:107:LYS:HG2   | 2.15                     | 0.47              |
| 2:M:1001:VAL:HG23 | 2:M:1002:GLU:N    | 2.29                     | 0.47              |
| 2:M:1063:ARG:O    | 2:M:1066:ALA:HB3  | 2.14                     | 0.47              |
| 2:M:237:ARG:O     | 2:M:240:THR:OG1   | 2.29                     | 0.47              |
| 2:M:273:GLY:HA2   | 2:M:276:LYS:NZ    | 2.30                     | 0.47              |
| 2:M:274:ARG:HH21  | 2:M:284:ARG:CB    | 2.10                     | 0.47              |
| 2:M:615:TYR:O     | 2:M:618:GLY:N     | 2.45                     | 0.47              |
| 1:K:22:GLU:OE1    | 2:M:934:PHE:CZ    | 2.67                     | 0.47              |
| 3:N:1221:VAL:HG12 | 3:N:1370:ILE:HD13 | 1.96                     | 0.47              |
| 3:N:1224:VAL:O    | 3:N:1225:ALA:C    | 2.52                     | 0.47              |
| 3:N:1223:ILE:O    | 3:N:1226:ALA:N    | 2.47                     | 0.47              |
| 3:N:1296:SER:C    | 3:N:1298:GLY:N    | 2.66                     | 0.47              |
| 3:N:1434:TRP:C    | 3:N:1434:TRP:CD1  | 2.86                     | 0.47              |
| 3:N:1436:SER:O    | 3:N:1439:SER:HB3  | 2.14                     | 0.47              |
| 3:N:368:VAL:HB    | 3:N:377:VAL:CB    | 2.44                     | 0.47              |
| 3:N:43:GLY:H      | 3:N:46:ASP:HB2    | 1.78                     | 0.47              |
| 3:N:497:GLU:HA    | 3:N:497:GLU:OE1   | 2.13                     | 0.47              |
| 3:N:73:CYS:C      | 3:N:75:ARG:H      | 2.18                     | 0.47              |
| 3:N:87:ARG:CA     | 3:N:523:ASP:HB2   | 2.43                     | 0.47              |
| 4:O:46:PRO:C      | 4:O:57:ASP:H      | 2.16                     | 0.47              |
| 4:O:70:THR:C      | 4:O:72:ARG:N      | 2.68                     | 0.47              |
| 5:P:353:GLU:HA    | 5:P:356:LYS:HB2   | 1.95                     | 0.47              |
| 1:B:5:LYS:HD3     | 1:B:5:LYS:HA      | 1.58                     | 0.47              |
| 2:C:1048:THR:O    | 2:C:1052:MET:CB   | 2.62                     | 0.47              |
| 2:C:191:PHE:HB2   | 2:C:192:PRO:CD    | 2.45                     | 0.47              |
| 2:C:246:ASP:CG    | 2:C:247:PRO:HD2   | 2.34                     | 0.47              |
| 2:C:334:ARG:HB2   | 2:C:339:LEU:CD2   | 2.42                     | 0.47              |
| 2:C:367:LEU:HG    | 2:C:372:LEU:CD2   | 2.38                     | 0.47              |
| 2:C:431:HIS:HE1   | 2:C:432:ARG:HG2   | 1.77                     | 0.47              |
| 2:C:471:TYR:O     | 2:C:484:VAL:N     | 2.47                     | 0.47              |
| 2:C:401:LEU:CD1   | 2:C:543:ASN:HB3   | 2.38                     | 0.47              |
| 2:C:575:GLN:HB2   | 2:C:670:GLN:HA    | 1.96                     | 0.47              |
| 2:C:615:TYR:OH    | 2:C:623:TYR:OH    | 2.26                     | 0.47              |
| 2:C:603:VAL:HG12  | 2:C:645:VAL:HA    | 1.96                     | 0.47              |
| 2:C:588:VAL:HG21  | 2:C:664:GLY:O     | 2.14                     | 0.47              |
| 2:C:78:PHE:HB3    | 2:C:79:PRO:HD2    | 1.95                     | 0.47              |
| 3:D:1016:PRO:O    | 3:D:1021:TYR:HD1  | 1.98                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:1095:THR:O   | 3:D:1096:ARG:C   | 2.53                     | 0.47              |
| 3:D:505:SER:CB   | 3:D:1453:ALA:O   | 2.62                     | 0.47              |
| 3:D:1465:ASN:ND2 | 3:D:1473:PRO:HD3 | 2.29                     | 0.47              |
| 3:D:315:ARG:HD2  | 3:D:315:ARG:N    | 2.27                     | 0.47              |
| 3:D:459:GLU:O    | 3:D:463:GLN:HG2  | 2.15                     | 0.47              |
| 3:D:55:ASP:HB3   | 3:D:82:LYS:HA    | 1.96                     | 0.47              |
| 3:D:582:LEU:HA   | 3:D:603:LEU:CD1  | 2.18                     | 0.47              |
| 3:D:656:PHE:H    | 3:D:656:PHE:HD1  | 1.62                     | 0.47              |
| 5:F:124:PRO:O    | 5:F:127:ILE:HB   | 2.14                     | 0.47              |
| 5:F:127:ILE:HG22 | 5:F:128:ARG:N    | 2.29                     | 0.47              |
| 5:F:209:PHE:CD2  | 5:F:213:ILE:HD11 | 2.50                     | 0.47              |
| 5:F:343:ASP:HB2  | 5:F:347:GLN:HE22 | 1.78                     | 0.47              |
| 5:F:411:HIS:C    | 5:F:413:SER:H    | 2.16                     | 0.47              |
| 5:F:95:THR:HG22  | 5:F:96:LEU:N     | 2.29                     | 0.47              |
| 1:K:133:GLU:HG2  | 1:K:134:GLU:N    | 2.29                     | 0.47              |
| 1:L:58:ILE:O     | 1:L:59:GLU:C     | 2.51                     | 0.47              |
| 2:M:408:ARG:O    | 2:M:454:SER:HA   | 2.15                     | 0.47              |
| 2:M:47:ALA:O     | 2:M:50:GLU:HG2   | 2.13                     | 0.47              |
| 2:M:540:PHE:CD1  | 2:M:540:PHE:N    | 2.82                     | 0.47              |
| 2:M:976:ASP:C    | 2:M:978:ARG:H    | 2.17                     | 0.47              |
| 3:N:1042:ARG:HB3 | 3:N:1057:VAL:CG1 | 2.44                     | 0.47              |
| 3:N:10:ILE:HG12  | 3:N:1451:ALA:HA  | 1.97                     | 0.47              |
| 3:N:1378:TYR:HB2 | 3:N:1422:MET:CE  | 2.43                     | 0.47              |
| 3:N:1489:GLN:O   | 3:N:1492:LEU:HB2 | 2.14                     | 0.47              |
| 3:N:227:LEU:HD11 | 3:N:326:GLU:HA   | 1.95                     | 0.47              |
| 3:N:207:PHE:HB2  | 3:N:391:ALA:H    | 1.79                     | 0.47              |
| 3:N:73:CYS:CB    | 3:N:76:CYS:SG    | 3.02                     | 0.47              |
| 3:N:843:PHE:HD1  | 3:N:848:GLU:OE2  | 1.96                     | 0.47              |
| 5:P:370:LYS:CG   | 5:P:371:LEU:N    | 2.70                     | 0.47              |
| 1:A:57:TYR:CE2   | 1:A:161:ARG:NH1  | 2.82                     | 0.47              |
| 1:B:78:ILE:HG22  | 1:B:82:LEU:HD21  | 1.96                     | 0.47              |
| 2:C:1004:LYS:HB3 | 2:C:1006:HIS:HE1 | 1.80                     | 0.47              |
| 2:C:97:ARG:HG2   | 2:C:111:ASP:HB3  | 1.96                     | 0.47              |
| 2:C:159:ILE:HG22 | 2:C:175:GLU:HB2  | 1.96                     | 0.47              |
| 2:C:185:LYS:CG   | 2:C:190:LYS:HD3  | 2.36                     | 0.47              |
| 2:C:327:HIS:ND1  | 2:C:329:GLY:N    | 2.62                     | 0.47              |
| 2:C:504:GLU:HG3  | 2:C:504:GLU:O    | 2.15                     | 0.47              |
| 2:C:512:ARG:CB   | 2:C:523:ILE:HD11 | 2.45                     | 0.47              |
| 2:C:527:GLU:N    | 2:C:527:GLU:OE1  | 2.47                     | 0.47              |
| 2:C:52:PHE:CD1   | 2:C:67:ASP:HA    | 2.48                     | 0.47              |
| 3:D:1001:GLU:CA  | 3:D:1001:GLU:OE2 | 2.56                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1253:THR:HG22 | 3:D:1254:GLN:H   | 1.80                     | 0.47              |
| 3:D:397:LYS:HG3   | 3:D:448:GLU:OE1  | 2.15                     | 0.47              |
| 3:D:401:TYR:HB2   | 3:D:444:VAL:HG23 | 1.95                     | 0.47              |
| 3:D:473:LEU:HA    | 3:D:476:GLU:HB3  | 1.96                     | 0.47              |
| 2:C:1090:LYS:HE3  | 3:D:88:TYR:O     | 2.15                     | 0.47              |
| 5:F:154:LYS:O     | 5:F:158:GLU:HG3  | 2.14                     | 0.47              |
| 1:K:143:ARG:NH1   | 1:K:158:ILE:HG23 | 2.29                     | 0.47              |
| 1:K:173:PRO:O     | 1:K:201:THR:HA   | 2.14                     | 0.47              |
| 1:L:88:ARG:HB2    | 1:L:121:GLU:HB3  | 1.96                     | 0.47              |
| 2:M:141:HIS:HE1   | 2:M:143:SER:HA   | 1.80                     | 0.47              |
| 2:M:209:ARG:HD2   | 2:M:209:ARG:N    | 2.28                     | 0.47              |
| 2:M:208:ALA:O     | 2:M:218:VAL:HG11 | 2.14                     | 0.47              |
| 2:M:276:LYS:CA    | 2:M:280:LYS:HE3  | 2.45                     | 0.47              |
| 2:M:322:VAL:O     | 2:M:323:ASP:CG   | 2.53                     | 0.47              |
| 2:M:544:THR:C     | 2:M:546:LEU:H    | 2.17                     | 0.47              |
| 2:M:693:GLU:HG3   | 2:M:697:ARG:HH11 | 1.79                     | 0.47              |
| 2:M:753:ASP:O     | 2:M:791:ARG:HA   | 2.14                     | 0.47              |
| 2:M:839:LEU:CD2   | 2:M:996:LYS:HA   | 2.32                     | 0.47              |
| 3:N:1489:GLN:HA   | 3:N:1492:LEU:HB2 | 1.96                     | 0.47              |
| 3:N:238:PRO:HB3   | 3:N:318:ARG:HA   | 1.96                     | 0.47              |
| 3:N:325:GLU:N     | 3:N:331:VAL:HG13 | 2.29                     | 0.47              |
| 3:N:508:ARG:HD3   | 3:N:510:GLU:OE1  | 2.14                     | 0.47              |
| 3:N:29:PRO:HG3    | 3:N:548:ILE:CG2  | 2.45                     | 0.47              |
| 3:N:58:CYS:SG     | 3:N:63:TYR:N     | 2.67                     | 0.47              |
| 2:M:1008:ARG:NH1  | 3:N:624:ASP:OD1  | 2.48                     | 0.47              |
| 3:N:644:LEU:HD12  | 3:N:645:PRO:CD   | 2.41                     | 0.47              |
| 3:N:812:ALA:C     | 3:N:814:ALA:H    | 2.16                     | 0.47              |
| 3:N:937:TYR:O     | 3:N:938:GLY:C    | 2.52                     | 0.47              |
| 4:O:46:PRO:HB3    | 4:O:57:ASP:HB3   | 1.94                     | 0.47              |
| 4:O:61:GLU:O      | 4:O:65:MET:HG3   | 2.14                     | 0.47              |
| 5:P:264:MET:O     | 5:P:267:THR:OG1  | 2.28                     | 0.47              |
| 1:A:206:THR:O     | 1:A:207:PRO:C    | 2.50                     | 0.47              |
| 1:A:76:VAL:O      | 1:A:80:LEU:HG    | 2.15                     | 0.47              |
| 2:C:1118:LYS:HG3  | 2:C:1119:ARG:N   | 2.29                     | 0.47              |
| 2:C:189:ARG:HH21  | 2:C:242:LEU:HD23 | 1.78                     | 0.47              |
| 2:C:431:HIS:HE1   | 2:C:433:THR:HG23 | 1.80                     | 0.47              |
| 2:C:448:ASN:HB3   | 2:C:452:ILE:HD12 | 1.95                     | 0.47              |
| 2:C:523:ILE:HG12  | 2:C:524:VAL:N    | 2.30                     | 0.47              |
| 2:C:893:ALA:HB1   | 2:C:897:LEU:HD12 | 1.96                     | 0.47              |
| 3:D:1025:GLN:C    | 3:D:1027:GLY:N   | 2.68                     | 0.47              |
| 3:D:102:ILE:C     | 3:D:104:PHE:N    | 2.68                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1293:PHE:HD1 | 3:D:1302:GLU:CA   | 2.27                     | 0.47              |
| 3:D:1397:LYS:CG  | 3:D:1398:TRP:HZ3  | 2.26                     | 0.47              |
| 3:D:254:GLU:OE1  | 3:D:299:GLU:HB2   | 2.15                     | 0.47              |
| 3:D:358:GLY:CA   | 3:D:385:VAL:O     | 2.59                     | 0.47              |
| 3:D:709:HIS:NE2  | 3:D:711:LEU:HB2   | 2.29                     | 0.47              |
| 2:C:1100:GLN:O   | 3:D:9:ARG:HB3     | 2.14                     | 0.47              |
| 5:F:368:VAL:CG2  | 5:F:369:LEU:N     | 2.71                     | 0.47              |
| 5:F:379:ARG:C    | 5:F:379:ARG:HD3   | 2.35                     | 0.47              |
| 1:L:34:VAL:C     | 1:L:36:LEU:H      | 2.18                     | 0.47              |
| 2:M:405:ARG:NH2  | 2:M:409:ARG:NE    | 2.63                     | 0.47              |
| 2:M:428:ARG:NH2  | 2:M:447:ALA:O     | 2.47                     | 0.47              |
| 2:M:489:THR:O    | 2:M:490:GLU:C     | 2.53                     | 0.47              |
| 2:M:605:LYS:HB2  | 2:M:610:ARG:HH21  | 1.79                     | 0.47              |
| 2:M:673:LEU:HD21 | 2:M:895:TYR:CD1   | 2.49                     | 0.47              |
| 2:M:777:ILE:HG22 | 5:P:409:LYS:HB3   | 1.96                     | 0.47              |
| 3:N:1103:HIS:CG  | 3:N:1104:GLU:N    | 2.82                     | 0.47              |
| 3:N:1121:PRO:O   | 3:N:1122:LEU:HD23 | 2.14                     | 0.47              |
| 3:N:1401:GLU:C   | 3:N:1403:LEU:H    | 2.17                     | 0.47              |
| 3:N:207:PHE:HD1  | 3:N:391:ALA:HB3   | 1.80                     | 0.47              |
| 3:N:79:GLU:CG    | 3:N:80:VAL:H      | 2.19                     | 0.47              |
| 3:N:866:VAL:N    | 3:N:873:LEU:O     | 2.40                     | 0.47              |
| 3:N:93:ILE:N     | 3:N:517:VAL:O     | 2.47                     | 0.47              |
| 3:N:970:LYS:HG3  | 3:N:974:ILE:CD1   | 2.44                     | 0.47              |
| 5:P:94:LEU:HD11  | 5:P:190:ALA:HB3   | 1.95                     | 0.47              |
| 5:P:373:LYS:HZ2  | 5:P:373:LYS:CB    | 2.26                     | 0.47              |
| 1:B:186:LEU:O    | 1:B:188:GLN:NE2   | 2.48                     | 0.47              |
| 3:D:135:LEU:HD11 | 3:D:148:GLU:CB    | 2.44                     | 0.47              |
| 3:D:139:GLY:HA2  | 3:D:450:TYR:HE2   | 1.79                     | 0.47              |
| 3:D:142:LEU:HB3  | 3:D:146:PRO:CA    | 2.37                     | 0.47              |
| 3:D:186:VAL:CG1  | 3:D:187:LYS:N     | 2.74                     | 0.47              |
| 3:D:358:GLY:HA2  | 3:D:385:VAL:CA    | 2.44                     | 0.47              |
| 3:D:545:ARG:O    | 3:D:546:ARG:C     | 2.52                     | 0.47              |
| 3:D:661:MET:HB3  | 3:D:667:ALA:HB2   | 1.95                     | 0.47              |
| 3:D:828:LYS:C    | 3:D:828:LYS:HE2   | 2.34                     | 0.47              |
| 3:D:833:GLU:O    | 3:D:834:THR:CG2   | 2.63                     | 0.47              |
| 4:E:29:GLN:HG3   | 4:E:30:LEU:N      | 2.30                     | 0.47              |
| 5:F:338:LEU:HA   | 5:F:339:PRO:HD3   | 1.75                     | 0.47              |
| 1:K:74:ASP:HB3   | 1:K:77:GLU:HB2    | 1.97                     | 0.47              |
| 1:L:159:LYS:HB2  | 1:L:164:ALA:HB3   | 1.97                     | 0.47              |
| 2:M:141:HIS:ND1  | 2:M:141:HIS:C     | 2.68                     | 0.47              |
| 2:M:396:ASP:O    | 2:M:403:SER:N     | 2.47                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:596:TYR:O     | 2:M:655:LEU:HD11 | 2.15                     | 0.47              |
| 2:M:650:ARG:CZ    | 2:M:653:ASP:OD1  | 2.63                     | 0.47              |
| 2:M:65:VAL:O      | 2:M:100:LEU:HD12 | 2.15                     | 0.47              |
| 2:M:726:ILE:O     | 2:M:728:HIS:N    | 2.47                     | 0.47              |
| 2:M:941:VAL:O     | 2:M:942:GLU:C    | 2.52                     | 0.47              |
| 3:N:954:ALA:HA    | 3:N:1039:CYS:SG  | 2.55                     | 0.47              |
| 3:N:1169:ASP:O    | 3:N:1170:ASP:C   | 2.51                     | 0.47              |
| 3:N:1313:VAL:CG2  | 3:N:1314:LYS:N   | 2.78                     | 0.47              |
| 3:N:1426:LYS:O    | 3:N:1429:LEU:N   | 2.47                     | 0.47              |
| 3:N:200:ASP:OD1   | 3:N:201:GLY:N    | 2.47                     | 0.47              |
| 4:O:56:ASP:HB3    | 4:O:63:TRP:HZ2   | 1.79                     | 0.47              |
| 4:O:90:GLU:O      | 4:O:94:PRO:HA    | 2.14                     | 0.47              |
| 5:P:300:ASP:HB3   | 5:P:302:LYS:HE3  | 1.96                     | 0.47              |
| 3:N:572:ARG:CD    | 5:P:80:PRO:HB3   | 2.44                     | 0.47              |
| 1:A:229:GLN:O     | 1:B:12:THR:HA    | 2.14                     | 0.47              |
| 1:B:112:ARG:CG    | 1:B:113:ASP:N    | 2.78                     | 0.47              |
| 1:B:117:VAL:CG1   | 1:B:118:ALA:H    | 2.27                     | 0.47              |
| 1:B:70:GLY:HA2    | 1:B:133:GLU:CG   | 2.45                     | 0.47              |
| 2:C:1118:LYS:HG3  | 2:C:1119:ARG:HG3 | 1.97                     | 0.47              |
| 2:C:431:HIS:CE1   | 2:C:433:THR:HG23 | 2.50                     | 0.47              |
| 2:C:737:LEU:HD22  | 2:C:754:ILE:CG2  | 2.44                     | 0.47              |
| 3:D:1067:VAL:HG22 | 3:D:1068:LEU:N   | 2.29                     | 0.47              |
| 3:D:111:LYS:O     | 3:D:115:LEU:HB2  | 2.15                     | 0.47              |
| 3:D:1280:VAL:HG13 | 3:D:1317:ASP:C   | 2.34                     | 0.47              |
| 3:D:441:ARG:O     | 3:D:443:VAL:HG23 | 2.15                     | 0.47              |
| 3:D:511:TRP:CE3   | 3:D:511:TRP:HA   | 2.49                     | 0.47              |
| 3:D:833:GLU:C     | 3:D:834:THR:HG23 | 2.34                     | 0.47              |
| 5:F:130:VAL:O     | 5:F:132:ARG:N    | 2.47                     | 0.47              |
| 5:F:269:ASN:O     | 5:F:271:LEU:N    | 2.47                     | 0.47              |
| 5:F:329:TYR:O     | 5:F:332:PHE:HD1  | 1.97                     | 0.47              |
| 1:K:66:SER:HB2    | 1:K:75:VAL:HG21  | 1.97                     | 0.47              |
| 1:L:18:ARG:O      | 1:L:207:PRO:HD3  | 2.15                     | 0.47              |
| 2:M:1046:ALA:HB1  | 3:N:1471:LEU:CD1 | 2.43                     | 0.47              |
| 2:M:1105:LYS:HB3  | 2:M:1107:ASN:ND2 | 2.29                     | 0.47              |
| 2:M:208:ALA:HB2   | 2:M:221:LEU:CD2  | 2.38                     | 0.47              |
| 2:M:252:LYS:CD    | 2:M:298:PHE:HE1  | 2.28                     | 0.47              |
| 2:M:431:HIS:ND1   | 2:M:432:ARG:N    | 2.62                     | 0.47              |
| 2:M:988:VAL:HG23  | 11:M:1123:HOH:O  | 2.15                     | 0.47              |
| 3:N:1011:PHE:HB3  | 3:N:1021:TYR:CD1 | 2.49                     | 0.47              |
| 3:N:1066:THR:HG22 | 3:N:1068:LEU:H   | 1.78                     | 0.47              |
| 3:N:1111:ASP:HA   | 3:N:1201:CYS:SG  | 2.54                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1174:LEU:O    | 3:N:1175:ILE:C    | 2.53                     | 0.47              |
| 3:N:1352:ILE:O    | 3:N:1353:GLN:C    | 2.53                     | 0.47              |
| 3:N:307:ALA:HB1   | 3:N:311:LEU:CD1   | 2.43                     | 0.47              |
| 3:N:783:ARG:HG2   | 3:N:783:ARG:HH11  | 1.79                     | 0.47              |
| 3:N:815:ALA:O     | 3:N:818:ARG:HB2   | 2.15                     | 0.47              |
| 3:N:857:ILE:O     | 3:N:858:VAL:CG2   | 2.63                     | 0.47              |
| 3:N:924:MET:HG3   | 3:N:925:GLU:N     | 2.30                     | 0.47              |
| 1:A:22:GLU:C      | 1:A:23:PHE:CD1    | 2.88                     | 0.47              |
| 1:B:58:ILE:HG22   | 1:B:61:VAL:HB     | 1.96                     | 0.47              |
| 1:B:74:ASP:OD2    | 1:B:75:VAL:N      | 2.47                     | 0.47              |
| 2:C:250:ARG:HB2   | 2:C:253:ALA:HB2   | 1.96                     | 0.47              |
| 2:C:523:ILE:O     | 2:C:524:VAL:CG1   | 2.62                     | 0.47              |
| 2:C:588:VAL:HG13  | 2:C:593:ALA:HB3   | 1.96                     | 0.47              |
| 2:C:731:GLU:C     | 2:C:733:ALA:H     | 2.17                     | 0.47              |
| 2:C:762:LYS:O     | 2:C:765:SER:N     | 2.47                     | 0.47              |
| 2:C:948:GLU:CB    | 2:C:953:VAL:HG23  | 2.44                     | 0.47              |
| 3:D:1009:LYS:O    | 3:D:1013:GLU:HG2  | 2.14                     | 0.47              |
| 3:D:1019:PRO:O    | 3:D:1020:LEU:C    | 2.52                     | 0.47              |
| 3:D:1172:HIS:O    | 3:D:1173:LEU:C    | 2.51                     | 0.47              |
| 3:D:1194:CYS:HB2  | 3:D:1204:CYS:CB   | 2.45                     | 0.47              |
| 3:D:1280:VAL:HG13 | 3:D:1317:ASP:N    | 2.30                     | 0.47              |
| 3:D:1397:LYS:C    | 3:D:1398:TRP:HE3  | 2.17                     | 0.47              |
| 3:D:1426:LYS:O    | 3:D:1429:LEU:HB3  | 2.14                     | 0.47              |
| 3:D:1462:LEU:O    | 3:D:1463:LYS:C    | 2.53                     | 0.47              |
| 3:D:833:GLU:O     | 3:D:834:THR:HG23  | 2.15                     | 0.47              |
| 3:D:988:ARG:NH2   | 3:D:1054:GLU:OE2  | 2.48                     | 0.47              |
| 4:E:5:GLY:O       | 4:E:9:LEU:N       | 2.36                     | 0.47              |
| 4:E:84:ARG:HG2    | 4:E:88:GLU:CG     | 2.45                     | 0.47              |
| 1:K:56:VAL:HG12   | 1:K:57:TYR:N      | 2.29                     | 0.47              |
| 1:L:5:LYS:NZ      | 1:L:189:ARG:CZ    | 2.77                     | 0.47              |
| 1:L:30:ARG:HA     | 1:L:193:ASP:OD1   | 2.14                     | 0.47              |
| 2:M:1038:TRP:HD1  | 2:M:1041:GLU:OE1  | 1.97                     | 0.47              |
| 2:M:342:ASP:O     | 2:M:346:VAL:HG13  | 2.15                     | 0.47              |
| 2:M:716:LYS:C     | 2:M:718:GLY:H     | 2.18                     | 0.47              |
| 2:M:727:PRO:HG2   | 2:M:785:VAL:O     | 2.15                     | 0.47              |
| 3:N:1124:GLN:O    | 3:N:1133:ARG:N    | 2.48                     | 0.47              |
| 3:N:1211:MET:HG3  | 3:N:1213:ARG:HH11 | 1.79                     | 0.47              |
| 3:N:1400:VAL:HA   | 3:N:1408:ILE:HD12 | 1.95                     | 0.47              |
| 3:N:1489:GLN:HA   | 3:N:1492:LEU:CD1  | 2.41                     | 0.47              |
| 3:N:329:GLU:HG2   | 3:N:330:THR:CG2   | 2.41                     | 0.47              |
| 3:N:554:LEU:CD1   | 3:N:558:LEU:HD11  | 2.45                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:O:6:ILE:HG23    | 4:O:7:ASP:N       | 2.30                     | 0.47              |
| 5:P:220:LEU:O     | 5:P:220:LEU:HD12  | 2.14                     | 0.47              |
| 5:P:234:LYS:HE2   | 5:P:236:SER:HB2   | 1.97                     | 0.47              |
| 2:C:1008:ARG:HD2  | 2:C:1028:GLY:C    | 2.36                     | 0.47              |
| 2:C:157:ARG:HH11  | 2:C:314:THR:HA    | 1.79                     | 0.47              |
| 2:C:191:PHE:HE2   | 2:C:196:LEU:HD21  | 1.76                     | 0.47              |
| 2:C:41:ASN:C      | 2:C:41:ASN:ND2    | 2.68                     | 0.47              |
| 2:C:517:ARG:HB2   | 2:C:520:GLU:CB    | 2.41                     | 0.47              |
| 3:D:1149:LEU:HG   | 3:D:1151:ARG:O    | 2.14                     | 0.47              |
| 3:D:1330:ILE:HD12 | 3:D:1347:TYR:CZ   | 2.49                     | 0.47              |
| 3:D:1462:LEU:O    | 3:D:1466:VAL:HG23 | 2.15                     | 0.47              |
| 3:D:212:ARG:HD3   | 3:D:342:PRO:HB3   | 1.97                     | 0.47              |
| 3:D:351:MET:HA    | 3:D:369:ALA:O     | 2.15                     | 0.47              |
| 3:D:592:THR:O     | 3:D:593:ASN:C     | 2.53                     | 0.47              |
| 3:D:832:ARG:C     | 3:D:834:THR:N     | 2.67                     | 0.47              |
| 3:D:843:PHE:CE1   | 3:D:849:ALA:HA    | 2.50                     | 0.47              |
| 3:D:944:THR:O     | 3:D:946:GLY:N     | 2.48                     | 0.47              |
| 5:F:386:VAL:HG12  | 5:F:394:ARG:N     | 2.30                     | 0.47              |
| 2:M:1014:SER:O    | 2:M:1018:GLN:N    | 2.46                     | 0.47              |
| 2:M:246:ASP:OD2   | 2:M:250:ARG:NH2   | 2.47                     | 0.47              |
| 2:M:262:ALA:O     | 2:M:265:ARG:HG2   | 2.15                     | 0.47              |
| 2:M:728:HIS:CD2   | 2:M:734:LEU:HD21  | 2.49                     | 0.47              |
| 1:K:22:GLU:OE1    | 2:M:934:PHE:HZ    | 1.97                     | 0.47              |
| 3:N:1109:GLU:HG3  | 3:N:1196:THR:HG23 | 1.97                     | 0.47              |
| 3:N:1311:LEU:CG   | 3:N:1312:LEU:N    | 2.78                     | 0.47              |
| 3:N:1342:GLU:O    | 3:N:1346:ARG:N    | 2.40                     | 0.47              |
| 3:N:1476:THR:CG2  | 4:O:20:THR:HB     | 2.45                     | 0.47              |
| 3:N:225:LEU:O     | 3:N:331:VAL:N     | 2.34                     | 0.47              |
| 3:N:554:LEU:HA    | 3:N:557:LEU:HD12  | 1.97                     | 0.47              |
| 3:N:601:ARG:HH11  | 3:N:601:ARG:HG2   | 1.79                     | 0.47              |
| 5:P:353:GLU:HG3   | 5:P:417:LYS:HD3   | 1.96                     | 0.47              |
| 5:P:382:THR:CG2   | 5:P:397:ILE:HB    | 2.45                     | 0.47              |
| 1:A:30:ARG:HH21   | 1:A:191:ASP:HB2   | 1.79                     | 0.47              |
| 1:B:238:GLU:HB3   | 1:B:240:LYS:NZ    | 2.29                     | 0.47              |
| 1:B:67:THR:OG1    | 1:B:68:ILE:N      | 2.47                     | 0.47              |
| 2:C:65:VAL:O      | 2:C:100:LEU:HD12  | 2.15                     | 0.47              |
| 2:C:1090:LYS:O    | 2:C:1091:GLU:C    | 2.53                     | 0.47              |
| 2:C:172:ILE:HG22  | 2:C:173:ASP:N     | 2.30                     | 0.47              |
| 2:C:176:VAL:O     | 2:C:178:PRO:HD3   | 2.14                     | 0.47              |
| 2:C:239:PHE:O     | 2:C:242:LEU:N     | 2.39                     | 0.47              |
| 2:C:24:GLU:O      | 2:C:25:SER:C      | 2.54                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:261:ILE:C    | 2:C:288:ARG:NH2   | 2.68                     | 0.47              |
| 2:C:264:PRO:CB   | 2:C:289:THR:HG21  | 2.42                     | 0.47              |
| 2:C:41:ASN:CA    | 2:C:45:GLN:HB3    | 2.28                     | 0.47              |
| 2:C:517:ARG:N    | 2:C:520:GLU:HB2   | 2.30                     | 0.47              |
| 2:C:3:ILE:HD11   | 2:C:5:ARG:HH21    | 1.79                     | 0.47              |
| 2:C:650:ARG:HE   | 2:C:650:ARG:H     | 0.79                     | 0.47              |
| 2:C:807:ARG:HH11 | 2:C:807:ARG:HB3   | 1.79                     | 0.47              |
| 3:D:1171:VAL:O   | 3:D:1172:HIS:C    | 2.52                     | 0.47              |
| 3:D:775:GLY:CA   | 3:D:1209:LEU:HD22 | 2.44                     | 0.47              |
| 3:D:1213:ARG:NH1 | 3:D:1213:ARG:HG2  | 2.23                     | 0.47              |
| 3:D:1442:ASN:ND2 | 3:D:1442:ASN:O    | 2.48                     | 0.47              |
| 3:D:1444:THR:O   | 3:D:1445:HIS:C    | 2.52                     | 0.47              |
| 3:D:164:GLY:HA3  | 3:D:447:VAL:HG12  | 1.97                     | 0.47              |
| 2:C:1056:LYS:HB3 | 3:D:623:VAL:HG13  | 1.97                     | 0.47              |
| 3:D:826:PRO:HB3  | 3:D:828:LYS:NZ    | 2.29                     | 0.47              |
| 5:F:102:LEU:CD1  | 5:F:183:ALA:HB1   | 2.45                     | 0.47              |
| 5:F:290:GLU:O    | 5:F:293:GLU:HB2   | 2.15                     | 0.47              |
| 5:F:313:GLU:CD   | 5:F:313:GLU:H     | 2.18                     | 0.47              |
| 1:L:111:ALA:HB3  | 1:L:125:PRO:CA    | 2.40                     | 0.47              |
| 1:L:87:VAL:HG12  | 1:L:122:ILE:HG12  | 1.96                     | 0.47              |
| 2:M:1105:LYS:CB  | 2:M:1107:ASN:ND2  | 2.78                     | 0.47              |
| 2:M:164:PRO:HD3  | 2:M:266:ARG:HH21  | 1.78                     | 0.47              |
| 2:M:257:VAL:HA   | 2:M:261:ILE:CD1   | 2.33                     | 0.47              |
| 2:M:264:PRO:C    | 2:M:289:THR:HG21  | 2.36                     | 0.47              |
| 2:M:439:CYS:HB2  | 2:M:541:SER:CB    | 2.43                     | 0.47              |
| 2:M:493:ARG:HB2  | 2:M:494:TYR:CD1   | 2.49                     | 0.47              |
| 2:M:760:SER:O    | 2:M:785:VAL:HG13  | 2.15                     | 0.47              |
| 2:M:906:PHE:HZ   | 3:N:1070:TYR:CG   | 2.33                     | 0.47              |
| 2:M:909:ALA:HA   | 2:M:913:GLU:OE1   | 2.15                     | 0.47              |
| 2:M:73:LEU:HB2   | 2:M:93:PRO:O      | 2.14                     | 0.47              |
| 3:N:1213:ARG:CG  | 3:N:1213:ARG:NH1  | 2.73                     | 0.47              |
| 3:N:1274:ILE:HA  | 3:N:1325:LEU:HG   | 1.96                     | 0.47              |
| 3:N:126:VAL:HG12 | 3:N:127:LEU:N     | 2.29                     | 0.47              |
| 3:N:1344:VAL:O   | 3:N:1347:TYR:HB3  | 2.14                     | 0.47              |
| 3:N:1496:GLU:OE2 | 3:N:1499:ARG:HB3  | 2.15                     | 0.47              |
| 3:N:188:GLY:N    | 3:N:198:ARG:HA    | 2.27                     | 0.47              |
| 3:N:224:ARG:HD2  | 3:N:332:TYR:HB2   | 1.97                     | 0.47              |
| 3:N:297:ILE:HB   | 3:N:302:GLN:HE22  | 1.80                     | 0.47              |
| 3:N:249:TYR:CG   | 3:N:307:ALA:HB3   | 2.49                     | 0.47              |
| 3:N:170:PRO:HA   | 3:N:391:ALA:O     | 2.14                     | 0.47              |
| 3:N:137:PRO:HD3  | 3:N:453:ASP:HB3   | 1.94                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:508:ARG:HA   | 3:N:509:PRO:HD2  | 1.63                     | 0.47              |
| 3:N:564:GLU:O    | 3:N:567:ILE:HB   | 2.15                     | 0.47              |
| 3:N:806:PHE:HA   | 3:N:809:PRO:CG   | 2.44                     | 0.47              |
| 5:P:247:ILE:O    | 5:P:248:ASN:C    | 2.51                     | 0.47              |
| 3:N:207:PHE:HE1  | 5:P:95:THR:HB    | 1.80                     | 0.47              |
| 2:C:93:PRO:HB3   | 2:C:114:PHE:HD1  | 1.80                     | 0.47              |
| 2:C:240:THR:C    | 2:C:242:LEU:N    | 2.68                     | 0.47              |
| 2:C:302:VAL:HB   | 2:C:303:PHE:HD1  | 1.79                     | 0.47              |
| 2:C:346:VAL:O    | 2:C:350:ARG:HG3  | 2.15                     | 0.47              |
| 2:C:408:ARG:HD3  | 11:C:1122:HOH:O  | 2.14                     | 0.47              |
| 2:C:441:VAL:O    | 2:C:559:LEU:HD13 | 2.15                     | 0.47              |
| 2:C:6:PHE:CB     | 2:C:908:GLY:HA2  | 2.44                     | 0.47              |
| 3:D:1296:SER:HB3 | 3:D:1299:PHE:HD1 | 1.80                     | 0.47              |
| 3:D:1404:ASN:HB3 | 3:D:1409:ALA:HB3 | 1.97                     | 0.47              |
| 3:D:416:ALA:CB   | 3:D:432:TYR:CG   | 2.97                     | 0.47              |
| 3:D:615:ARG:O    | 3:D:1096:ARG:NH2 | 2.48                     | 0.47              |
| 2:C:1043:TYR:CD1 | 3:D:710:ARG:HB2  | 2.50                     | 0.47              |
| 3:D:87:ARG:HG3   | 3:D:88:TYR:CD2   | 2.50                     | 0.47              |
| 3:D:932:ASP:CA   | 3:D:935:LYS:HE2  | 2.45                     | 0.47              |
| 2:C:889:HIS:CE1  | 3:D:951:ILE:H    | 2.24                     | 0.47              |
| 4:E:42:PRO:O     | 4:E:43:GLU:C     | 2.54                     | 0.47              |
| 5:F:111:GLU:O    | 5:F:114:LYS:HB2  | 2.15                     | 0.47              |
| 5:F:393:THR:HG22 | 5:F:395:GLU:H    | 1.80                     | 0.47              |
| 1:K:200:TRP:CD1  | 1:K:200:TRP:N    | 2.83                     | 0.47              |
| 2:M:175:GLU:C    | 2:M:183:SER:HB2  | 2.35                     | 0.47              |
| 2:M:175:GLU:CG   | 2:M:176:VAL:H    | 2.11                     | 0.47              |
| 2:M:399:ASN:O    | 2:M:402:SER:OG   | 2.28                     | 0.47              |
| 2:M:800:VAL:HG12 | 2:M:801:VAL:N    | 2.30                     | 0.47              |
| 2:M:928:LYS:O    | 2:M:929:ARG:C    | 2.54                     | 0.47              |
| 2:M:918:LEU:CD1  | 2:M:968:LEU:HA   | 2.45                     | 0.47              |
| 3:N:1041:LEU:HG  | 3:N:1043:GLY:N   | 2.29                     | 0.47              |
| 3:N:1084:THR:O   | 3:N:1085:ALA:C   | 2.53                     | 0.47              |
| 3:N:1104:GLU:OE1 | 3:N:1104:GLU:N   | 2.47                     | 0.47              |
| 3:N:114:THR:O    | 3:N:114:THR:HG22 | 2.15                     | 0.47              |
| 3:N:1380:GLU:HA  | 3:N:1392:GLY:HA2 | 1.97                     | 0.47              |
| 3:N:274:ARG:HD3  | 3:N:279:VAL:HG11 | 1.97                     | 0.47              |
| 3:N:403:PHE:HD1  | 3:N:423:ASP:OD1  | 1.96                     | 0.47              |
| 3:N:692:GLU:C    | 3:N:692:GLU:CD   | 2.74                     | 0.47              |
| 5:P:102:LEU:HD21 | 5:P:187:LEU:N    | 2.30                     | 0.47              |
| 5:P:145:PRO:HB2  | 5:P:150:THR:H    | 1.79                     | 0.47              |
| 5:P:271:LEU:O    | 5:P:272:SER:C    | 2.52                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:P:321:ILE:HD11 | 5:P:329:TYR:CA    | 2.45                     | 0.47              |
| 5:P:352:GLU:C    | 5:P:354:LEU:N     | 2.66                     | 0.47              |
| 1:A:71:VAL:HG22  | 1:A:132:LEU:CD2   | 2.45                     | 0.46              |
| 1:B:179:PHE:CB   | 1:B:197:LEU:HD13  | 2.28                     | 0.46              |
| 1:B:217:ILE:HG22 | 1:B:221:HIS:NE2   | 2.30                     | 0.46              |
| 1:B:24:VAL:HG12  | 1:B:25:LEU:N      | 2.30                     | 0.46              |
| 2:C:191:PHE:CD2  | 2:C:192:PRO:O     | 2.68                     | 0.46              |
| 2:C:144:PRO:O    | 2:C:266:ARG:HD3   | 2.14                     | 0.46              |
| 2:C:548:PRO:HG2  | 2:C:843:HIS:CE1   | 2.50                     | 0.46              |
| 3:D:1403:LEU:HB3 | 3:D:1408:ILE:HD12 | 1.97                     | 0.46              |
| 3:D:368:VAL:N    | 3:D:377:VAL:HB    | 2.27                     | 0.46              |
| 3:D:739:ASP:N    | 3:D:739:ASP:OD1   | 2.42                     | 0.46              |
| 3:D:747:VAL:HG22 | 3:D:748:HIS:N     | 2.30                     | 0.46              |
| 5:F:112:ALA:O    | 5:F:113:ILE:C     | 2.53                     | 0.46              |
| 5:F:90:GLN:OE1   | 5:F:189:GLU:HB3   | 2.15                     | 0.46              |
| 1:L:95:GLN:O     | 1:L:145:ASP:OD1   | 2.32                     | 0.46              |
| 2:M:1090:LYS:O   | 2:M:1094:ALA:N    | 2.35                     | 0.46              |
| 2:M:200:LEU:HB2  | 2:M:202:TYR:CE2   | 2.50                     | 0.46              |
| 2:M:304:LEU:O    | 2:M:308:ARG:HG2   | 2.15                     | 0.46              |
| 2:M:550:LEU:C    | 2:M:552:HIS:H     | 2.18                     | 0.46              |
| 2:M:583:LEU:O    | 2:M:587:VAL:HG23  | 2.15                     | 0.46              |
| 3:N:1033:GLN:O   | 3:N:1034:GLN:C    | 2.52                     | 0.46              |
| 3:N:1079:LYS:HB3 | 3:N:1239:ARG:NH2  | 2.30                     | 0.46              |
| 3:N:257:GLY:CA   | 3:N:274:ARG:CA    | 2.92                     | 0.46              |
| 3:N:440:VAL:HG23 | 3:N:441:ARG:N     | 2.30                     | 0.46              |
| 3:N:131:LYS:C    | 3:N:456:MET:HE3   | 2.36                     | 0.46              |
| 3:N:470:LEU:HB2  | 3:N:503:LEU:HG    | 1.97                     | 0.46              |
| 3:N:750:PRO:HG2  | 3:N:756:GLN:NE2   | 2.31                     | 0.46              |
| 3:N:788:GLY:N    | 3:N:942:SER:HB3   | 2.30                     | 0.46              |
| 3:N:879:ARG:HB3  | 3:N:902:LEU:HD12  | 1.97                     | 0.46              |
| 3:N:87:ARG:HA    | 3:N:523:ASP:HB2   | 1.97                     | 0.46              |
| 4:O:19:LEU:O     | 4:O:23:VAL:HG23   | 2.15                     | 0.46              |
| 4:O:40:LEU:HD13  | 4:O:72:ARG:CZ     | 2.45                     | 0.46              |
| 5:P:216:GLY:HA3  | 5:P:243:ILE:HG23  | 1.97                     | 0.46              |
| 5:P:279:GLN:HA   | 5:P:286:PRO:HD3   | 1.97                     | 0.46              |
| 5:P:282:LEU:C    | 5:P:284:ARG:N     | 2.69                     | 0.46              |
| 5:P:300:ASP:CB   | 5:P:302:LYS:HE3   | 2.45                     | 0.46              |
| 1:A:218:LEU:O    | 1:A:221:HIS:HB2   | 2.15                     | 0.46              |
| 1:B:54:THR:O     | 1:B:167:VAL:N     | 2.48                     | 0.46              |
| 1:B:175:ARG:O    | 1:B:176:ARG:HB2   | 2.13                     | 0.46              |
| 1:B:233:VAL:C    | 1:B:235:ALA:N     | 2.68                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:1000:MET:O   | 2:C:1003:ASP:N    | 2.47                     | 0.46              |
| 2:C:1102:LEU:CD2 | 2:C:1108:PRO:HA   | 2.45                     | 0.46              |
| 2:C:1112:PHE:C   | 2:C:1113:GLU:HG2  | 2.35                     | 0.46              |
| 2:C:204:GLN:HE22 | 2:C:225:SER:HB3   | 1.81                     | 0.46              |
| 2:C:260:LEU:HD12 | 2:C:288:ARG:NE    | 2.30                     | 0.46              |
| 2:C:769:PRO:HA   | 2:C:772:ARG:HB2   | 1.96                     | 0.46              |
| 2:C:910:LYS:CG   | 2:C:913:GLU:HG3   | 2.34                     | 0.46              |
| 2:C:916:GLU:C    | 2:C:916:GLU:OE1   | 2.54                     | 0.46              |
| 3:D:1122:LEU:O   | 3:D:1135:ARG:N    | 2.47                     | 0.46              |
| 3:D:126:VAL:CG1  | 3:D:132:TYR:HB2   | 2.45                     | 0.46              |
| 3:D:1399:ASP:O   | 3:D:1403:LEU:CB   | 2.63                     | 0.46              |
| 3:D:1434:TRP:CZ3 | 3:D:1457:ASP:N    | 2.82                     | 0.46              |
| 3:D:414:ARG:NH1  | 3:D:451:ASP:OD2   | 2.48                     | 0.46              |
| 3:D:511:TRP:HE3  | 3:D:511:TRP:HA    | 1.79                     | 0.46              |
| 3:D:567:ILE:O    | 3:D:568:ARG:C     | 2.53                     | 0.46              |
| 5:F:110:MET:CE   | 5:F:111:GLU:HG3   | 2.45                     | 0.46              |
| 1:K:107:LYS:HE3  | 1:K:107:LYS:HB2   | 1.65                     | 0.46              |
| 1:K:11:PHE:CD1   | 1:L:225:PHE:HA    | 2.50                     | 0.46              |
| 1:L:152:PRO:HG2  | 1:L:155:LYS:CB    | 2.45                     | 0.46              |
| 1:L:161:ARG:HB2  | 1:L:164:ALA:CB    | 2.29                     | 0.46              |
| 2:M:141:HIS:HD2  | 2:M:334:ARG:HG3   | 1.80                     | 0.46              |
| 2:M:305:PRO:CA   | 2:M:308:ARG:HG2   | 2.44                     | 0.46              |
| 2:M:551:GLU:O    | 3:N:1064:GLY:HA2  | 2.15                     | 0.46              |
| 3:N:1048:PRO:HA  | 3:N:1079:LYS:CE   | 2.45                     | 0.46              |
| 3:N:1092:GLY:O   | 3:N:1096:ARG:HB2  | 2.15                     | 0.46              |
| 3:N:1147:ARG:HD2 | 3:N:1188:VAL:HG21 | 1.97                     | 0.46              |
| 3:N:1339:LYS:HB3 | 3:N:1343:ALA:HB2  | 1.96                     | 0.46              |
| 3:N:1400:VAL:O   | 3:N:1408:ILE:HD12 | 2.15                     | 0.46              |
| 3:N:528:VAL:O    | 3:N:535:PHE:HB3   | 2.14                     | 0.46              |
| 3:N:740:PHE:N    | 3:N:740:PHE:CD1   | 2.82                     | 0.46              |
| 3:N:932:ASP:O    | 3:N:933:ALA:C     | 2.54                     | 0.46              |
| 5:P:260:ILE:CG1  | 5:P:261:PRO:HD2   | 2.44                     | 0.46              |
| 5:P:306:GLU:CD   | 5:P:306:GLU:N     | 2.69                     | 0.46              |
| 5:P:308:LEU:O    | 5:P:311:ALA:N     | 2.41                     | 0.46              |
| 5:P:373:LYS:HD2  | 5:P:374:GLY:CA    | 2.44                     | 0.46              |
| 5:P:386:VAL:CG1  | 5:P:394:ARG:N     | 2.77                     | 0.46              |
| 5:P:392:VAL:CG1  | 5:P:396:ARG:HD3   | 2.42                     | 0.46              |
| 1:A:169:ALA:HB1  | 1:A:171:PHE:CZ    | 2.50                     | 0.46              |
| 1:B:28:LEU:HA    | 1:B:28:LEU:HD23   | 1.69                     | 0.46              |
| 1:B:32:PHE:O     | 1:B:36:LEU:N      | 2.47                     | 0.46              |
| 2:C:186:VAL:HG22 | 2:C:189:ARG:O     | 2.15                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:243:ARG:HG2   | 2:C:244:PRO:HG3   | 1.96                     | 0.46              |
| 2:C:448:ASN:HA    | 2:C:451:LEU:HD12  | 1.96                     | 0.46              |
| 2:C:517:ARG:O     | 2:C:520:GLU:CG    | 2.63                     | 0.46              |
| 2:C:594:ALA:C     | 2:C:595:LEU:HD23  | 2.35                     | 0.46              |
| 2:C:71:TYR:CD2    | 2:C:71:TYR:N      | 2.69                     | 0.46              |
| 2:C:832:LYS:CG    | 2:C:833:LEU:H     | 2.28                     | 0.46              |
| 3:D:1290:LEU:O    | 3:D:1305:LEU:HD23 | 2.14                     | 0.46              |
| 3:D:1426:LYS:O    | 3:D:1427:SER:C    | 2.54                     | 0.46              |
| 3:D:168:THR:HB    | 3:D:206:ARG:CZ    | 2.45                     | 0.46              |
| 3:D:274:ARG:HE    | 3:D:279:VAL:CG1   | 2.27                     | 0.46              |
| 3:D:246:PRO:HD2   | 3:D:308:LYS:HA    | 1.96                     | 0.46              |
| 3:D:558:LEU:C     | 3:D:560:GLN:H     | 2.18                     | 0.46              |
| 3:D:866:VAL:HG12  | 3:D:867:ARG:N     | 2.30                     | 0.46              |
| 3:D:991:GLN:HA    | 3:D:994:GLN:HG2   | 1.98                     | 0.46              |
| 4:E:19:LEU:HD12   | 4:E:19:LEU:O      | 2.16                     | 0.46              |
| 4:E:39:VAL:HG23   | 4:E:67:GLU:OE2    | 2.15                     | 0.46              |
| 4:E:61:GLU:O      | 4:E:62:THR:C      | 2.53                     | 0.46              |
| 5:F:100:VAL:O     | 5:F:103:ALA:HB3   | 2.15                     | 0.46              |
| 5:F:323:ASP:O     | 5:F:325:LYS:HG3   | 2.14                     | 0.46              |
| 1:K:202:ASP:OD1   | 1:K:203:GLY:N     | 2.48                     | 0.46              |
| 1:K:206:THR:N     | 1:K:209:GLU:OE1   | 2.47                     | 0.46              |
| 1:L:161:ARG:N     | 1:L:164:ALA:HB2   | 2.29                     | 0.46              |
| 1:L:208:LEU:O     | 1:L:209:GLU:C     | 2.54                     | 0.46              |
| 1:L:18:ARG:NH1    | 1:L:88:ARG:HH22   | 2.04                     | 0.46              |
| 2:M:1118:LYS:O    | 2:M:1119:ARG:HB2  | 2.13                     | 0.46              |
| 2:M:305:PRO:O     | 2:M:306:THR:C     | 2.53                     | 0.46              |
| 2:M:562:SER:O     | 2:M:565:GLN:N     | 2.48                     | 0.46              |
| 2:M:757:GLY:HA2   | 2:M:789:SER:HB3   | 1.96                     | 0.46              |
| 3:N:1353:GLN:O    | 3:N:1354:LYS:C    | 2.53                     | 0.46              |
| 3:N:1363:LEU:HD23 | 3:N:1364:HIS:N    | 2.30                     | 0.46              |
| 3:N:149:LYS:CG    | 3:N:150:ARG:N     | 2.78                     | 0.46              |
| 3:N:264:LEU:HB2   | 3:N:267:GLY:H     | 1.77                     | 0.46              |
| 3:N:224:ARG:CG    | 3:N:330:THR:OG1   | 2.63                     | 0.46              |
| 3:N:759:ALA:HA    | 3:N:763:MET:SD    | 2.55                     | 0.46              |
| 3:N:765:SER:C     | 3:N:767:HIS:H     | 2.18                     | 0.46              |
| 3:N:864:VAL:CG1   | 3:N:865:THR:H     | 2.19                     | 0.46              |
| 3:N:760:ARG:NH1   | 4:O:59:ASN:OD1    | 2.48                     | 0.46              |
| 4:O:68:LEU:O      | 4:O:69:LEU:C      | 2.52                     | 0.46              |
| 5:P:265:VAL:O     | 5:P:268:ILE:HB    | 2.14                     | 0.46              |
| 5:P:381:HIS:C     | 5:P:385:GLU:HG3   | 2.36                     | 0.46              |
| 1:A:154:GLU:N     | 1:A:154:GLU:CD    | 2.62                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1017:THR:O    | 2:C:1018:GLN:HB2 | 2.15                     | 0.46              |
| 2:C:233:GLU:O     | 2:C:237:ARG:HG3  | 2.16                     | 0.46              |
| 2:C:141:HIS:HD2   | 2:C:334:ARG:HG2  | 1.81                     | 0.46              |
| 2:C:453:THR:OG1   | 2:C:454:SER:N    | 2.48                     | 0.46              |
| 2:C:543:ASN:HB2   | 2:C:565:GLN:HE21 | 1.80                     | 0.46              |
| 3:D:1066:THR:HG22 | 3:D:1067:VAL:N   | 2.30                     | 0.46              |
| 3:D:1098:LEU:CD1  | 3:D:1098:LEU:N   | 2.76                     | 0.46              |
| 3:D:1341:PRO:O    | 3:D:1342:GLU:C   | 2.53                     | 0.46              |
| 3:D:142:LEU:CB    | 3:D:146:PRO:HA   | 2.39                     | 0.46              |
| 3:D:22:SER:C      | 3:D:24:GLY:H     | 2.19                     | 0.46              |
| 3:D:379:ALA:C     | 3:D:380:GLU:HG3  | 2.35                     | 0.46              |
| 3:D:206:ARG:NE    | 3:D:394:LEU:HB2  | 2.10                     | 0.46              |
| 3:D:499:VAL:HG12  | 3:D:503:LEU:CD1  | 2.45                     | 0.46              |
| 3:D:562:ALA:HB1   | 3:D:566:ILE:HD11 | 1.97                     | 0.46              |
| 3:D:592:THR:HG22  | 3:D:600:LEU:HD21 | 1.98                     | 0.46              |
| 3:D:692:GLU:O     | 3:D:695:ILE:N    | 2.49                     | 0.46              |
| 4:E:27:ALA:O      | 4:E:28:GLN:C     | 2.54                     | 0.46              |
| 4:E:30:LEU:CD1    | 4:E:37:ASN:HB2   | 2.45                     | 0.46              |
| 5:F:274:THR:HG22  | 5:F:278:LEU:CG   | 2.45                     | 0.46              |
| 5:F:371:LEU:HD23  | 5:F:375:LEU:CD1  | 2.46                     | 0.46              |
| 1:K:125:PRO:HG2   | 1:K:126:ASP:H    | 1.80                     | 0.46              |
| 1:K:56:VAL:O      | 1:K:165:ILE:N    | 2.49                     | 0.46              |
| 1:K:41:ARG:HA     | 1:K:177:VAL:HG11 | 1.97                     | 0.46              |
| 1:K:182:GLU:HG2   | 1:K:194:LYS:O    | 2.15                     | 0.46              |
| 1:K:41:ARG:HG2    | 1:K:45:LEU:CD1   | 2.45                     | 0.46              |
| 1:K:75:VAL:HA     | 1:K:78:ILE:HD12  | 1.97                     | 0.46              |
| 1:L:143:ARG:HG3   | 1:L:143:ARG:HH11 | 1.81                     | 0.46              |
| 1:L:180:GLN:O     | 1:L:180:GLN:HG2  | 2.15                     | 0.46              |
| 1:L:200:TRP:N     | 1:L:200:TRP:CD1  | 2.83                     | 0.46              |
| 1:K:34:VAL:CG1    | 1:L:42:ARG:NH1   | 2.78                     | 0.46              |
| 2:M:1045:ALA:HB1  | 2:M:1048:THR:OG1 | 2.15                     | 0.46              |
| 2:M:143:SER:HB3   | 2:M:332:ARG:HB2  | 1.97                     | 0.46              |
| 2:M:261:ILE:CA    | 2:M:288:ARG:HH21 | 2.29                     | 0.46              |
| 2:M:48:PHE:O      | 2:M:50:GLU:N     | 2.48                     | 0.46              |
| 2:M:631:SER:HB2   | 2:M:637:LEU:HD11 | 1.96                     | 0.46              |
| 2:M:53:PRO:HB3    | 2:M:67:ASP:OD2   | 2.15                     | 0.46              |
| 1:L:30:ARG:HD3    | 2:M:854:PRO:HG3  | 1.98                     | 0.46              |
| 3:N:1048:PRO:HA   | 3:N:1079:LYS:HZ1 | 1.79                     | 0.46              |
| 3:N:1079:LYS:HA   | 3:N:1082:ALA:HB3 | 1.98                     | 0.46              |
| 3:N:1206:GLY:O    | 3:N:1214:PRO:HA  | 2.15                     | 0.46              |
| 3:N:1236:LEU:O    | 3:N:1237:THR:C   | 2.53                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1258:ARG:HH21 | 3:N:1351:GLU:HG3 | 1.81                     | 0.46              |
| 3:N:1466:VAL:C    | 3:N:1468:LEU:N   | 2.69                     | 0.46              |
| 3:N:1481:VAL:O    | 3:N:1482:ARG:C   | 2.53                     | 0.46              |
| 3:N:149:LYS:N     | 3:N:149:LYS:CD   | 2.76                     | 0.46              |
| 3:N:172:PRO:O     | 3:N:173:PRO:C    | 2.54                     | 0.46              |
| 3:N:234:GLU:C     | 3:N:236:TYR:H    | 2.19                     | 0.46              |
| 3:N:324:ALA:HA    | 3:N:333:LEU:HD23 | 1.97                     | 0.46              |
| 3:N:490:ALA:HA    | 3:N:493:ARG:HH21 | 1.80                     | 0.46              |
| 4:O:60:ALA:O      | 4:O:61:GLU:C     | 2.53                     | 0.46              |
| 5:P:319:THR:HA    | 5:P:320:PRO:HD3  | 1.82                     | 0.46              |
| 5:P:352:GLU:O     | 5:P:355:GLU:CD   | 2.54                     | 0.46              |
| 1:A:110:LYS:HA    | 1:A:127:LEU:O    | 2.15                     | 0.46              |
| 1:A:195:LEU:HD12  | 1:A:195:LEU:C    | 2.35                     | 0.46              |
| 1:A:91:ASN:O      | 1:A:94:LEU:HB2   | 2.16                     | 0.46              |
| 1:B:208:LEU:O     | 1:B:211:LEU:N    | 2.48                     | 0.46              |
| 2:C:56:GLU:O      | 2:C:359:MET:HE1  | 2.16                     | 0.46              |
| 2:C:75:GLU:O      | 2:C:77:PRO:HD3   | 2.16                     | 0.46              |
| 2:C:807:ARG:O     | 2:C:809:GLY:N    | 2.49                     | 0.46              |
| 3:D:1018:ASN:C    | 3:D:1018:ASN:OD1 | 2.53                     | 0.46              |
| 3:D:1137:ARG:C    | 3:D:1141:GLU:HG3 | 2.36                     | 0.46              |
| 3:D:1312:LEU:HG   | 3:D:1312:LEU:O   | 2.16                     | 0.46              |
| 3:D:1341:PRO:HB2  | 3:D:1342:GLU:OE1 | 2.14                     | 0.46              |
| 3:D:1344:VAL:CG1  | 3:D:1345:GLU:H   | 2.28                     | 0.46              |
| 3:D:434:ARG:HH21  | 3:D:451:ASP:HA   | 1.81                     | 0.46              |
| 3:D:567:ILE:HG22  | 3:D:571:LYS:CE   | 2.43                     | 0.46              |
| 2:C:1070:ILE:HG21 | 3:D:656:PHE:CE1  | 2.51                     | 0.46              |
| 3:D:656:PHE:O     | 3:D:659:LYS:HB3  | 2.16                     | 0.46              |
| 3:D:680:GLN:HA    | 3:D:683:ILE:CG1  | 2.45                     | 0.46              |
| 3:D:917:GLN:O     | 3:D:918:ALA:C    | 2.54                     | 0.46              |
| 3:D:995:LEU:O     | 3:D:998:GLU:HB3  | 2.15                     | 0.46              |
| 4:E:50:THR:O      | 4:E:51:LEU:HB2   | 2.15                     | 0.46              |
| 3:D:1498:ALA:HB3  | 4:E:84:ARG:CZ    | 2.45                     | 0.46              |
| 5:F:265:VAL:N     | 5:F:268:ILE:HD12 | 2.30                     | 0.46              |
| 5:F:288:TYR:O     | 5:F:289:GLU:C    | 2.53                     | 0.46              |
| 5:F:353:GLU:HA    | 5:F:356:LYS:HB2  | 1.97                     | 0.46              |
| 1:L:217:ILE:HG22  | 1:L:221:HIS:CD2  | 2.51                     | 0.46              |
| 2:M:1085:PHE:CZ   | 3:N:1468:LEU:HG  | 2.50                     | 0.46              |
| 2:M:172:ILE:CG2   | 2:M:173:ASP:N    | 2.78                     | 0.46              |
| 2:M:539:VAL:O     | 2:M:539:VAL:HG12 | 2.15                     | 0.46              |
| 3:N:1038:LEU:O    | 3:N:1060:SER:HB2 | 2.16                     | 0.46              |
| 3:N:1091:SER:O    | 3:N:1092:GLY:C   | 2.54                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1311:LEU:HG   | 3:N:1313:VAL:H    | 1.80                     | 0.46              |
| 3:N:438:ASP:CG    | 3:N:439:LEU:H     | 2.19                     | 0.46              |
| 3:N:539:ASP:O     | 3:N:540:LEU:C     | 2.54                     | 0.46              |
| 2:M:1056:LYS:CE   | 3:N:625:TYR:HB2   | 2.32                     | 0.46              |
| 3:N:637:LEU:HD13  | 3:N:642:CYS:HA    | 1.97                     | 0.46              |
| 3:N:661:MET:CE    | 3:N:677:LEU:HD11  | 2.44                     | 0.46              |
| 3:N:765:SER:O     | 3:N:767:HIS:N     | 2.47                     | 0.46              |
| 3:N:799:LYS:HB2   | 3:N:826:PRO:CD    | 2.46                     | 0.46              |
| 5:P:223:ALA:HB2   | 5:P:242:TRP:CG    | 2.50                     | 0.46              |
| 5:P:291:ILE:O     | 5:P:294:ALA:N     | 2.49                     | 0.46              |
| 1:A:209:GLU:CA    | 1:A:212:ASN:ND2   | 2.79                     | 0.46              |
| 1:B:144:VAL:HG12  | 1:B:145:ASP:H     | 1.81                     | 0.46              |
| 1:B:52:ALA:HB3    | 1:B:171:PHE:CD2   | 2.51                     | 0.46              |
| 1:B:195:LEU:HD12  | 1:B:196:THR:N     | 2.30                     | 0.46              |
| 1:B:70:GLY:C      | 1:B:133:GLU:HG2   | 2.36                     | 0.46              |
| 2:C:12:VAL:HG12   | 2:C:481:ASP:OD1   | 2.15                     | 0.46              |
| 2:C:218:VAL:O     | 2:C:221:LEU:HB3   | 2.16                     | 0.46              |
| 2:C:238:LEU:O     | 2:C:241:LEU:CG    | 2.52                     | 0.46              |
| 2:C:239:PHE:O     | 2:C:240:THR:C     | 2.53                     | 0.46              |
| 2:C:626:ARG:HH11  | 2:C:626:ARG:CG    | 2.26                     | 0.46              |
| 2:C:707:ARG:NH2   | 2:C:709:GLU:OE2   | 2.48                     | 0.46              |
| 2:C:808:ARG:O     | 2:C:809:GLY:C     | 2.53                     | 0.46              |
| 2:C:674:VAL:CA    | 2:C:869:VAL:HG13  | 2.46                     | 0.46              |
| 2:C:910:LYS:HE3   | 2:C:912:PRO:CB    | 2.45                     | 0.46              |
| 2:C:941:VAL:O     | 2:C:942:GLU:C     | 2.53                     | 0.46              |
| 3:D:1041:LEU:HG   | 3:D:1043:GLY:H    | 1.76                     | 0.46              |
| 3:D:1114:THR:O    | 3:D:1114:THR:HG23 | 2.16                     | 0.46              |
| 3:D:1120:VAL:CB   | 3:D:1144:LEU:HD21 | 2.45                     | 0.46              |
| 3:D:1155:VAL:O    | 3:D:1158:VAL:N    | 2.28                     | 0.46              |
| 3:D:1172:HIS:CA   | 3:D:1175:ILE:HD12 | 2.33                     | 0.46              |
| 3:D:1480:PHE:HD2  | 3:D:1481:VAL:HG23 | 1.72                     | 0.46              |
| 3:D:246:PRO:O     | 3:D:248:PRO:HA    | 2.15                     | 0.46              |
| 3:D:32:ILE:HG23   | 3:D:38:LYS:N      | 2.31                     | 0.46              |
| 3:D:418:GLY:O     | 3:D:428:LYS:CE    | 2.63                     | 0.46              |
| 3:D:470:LEU:C     | 3:D:472:ALA:N     | 2.67                     | 0.46              |
| 3:D:769:LEU:N     | 3:D:769:LEU:HD12  | 2.30                     | 0.46              |
| 3:D:907:GLU:H     | 3:D:910:SER:HG    | 1.64                     | 0.46              |
| 2:C:984:GLU:CG    | 3:D:944:THR:O     | 2.64                     | 0.46              |
| 5:F:207:LEU:C     | 5:F:212:LEU:HD21  | 2.35                     | 0.46              |
| 5:F:270:LYS:HA    | 5:F:273:ARG:HD2   | 1.98                     | 0.46              |
| 2:C:1015:LEU:HD12 | 5:F:335:ASP:CB    | 2.46                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:F:361:LEU:HG    | 5:F:362:SER:H    | 1.79                     | 0.46              |
| 2:M:370:ALA:O     | 2:M:373:VAL:N    | 2.38                     | 0.46              |
| 2:M:415:PRO:C     | 2:M:417:GLY:H    | 2.19                     | 0.46              |
| 2:M:906:PHE:CZ    | 3:N:1070:TYR:CD2 | 3.04                     | 0.46              |
| 2:M:946:ARG:NH1   | 2:M:984:GLU:CB   | 2.79                     | 0.46              |
| 3:N:106:LYS:O     | 3:N:108:VAL:HG12 | 2.15                     | 0.46              |
| 3:N:1444:THR:O    | 3:N:1445:HIS:C   | 2.54                     | 0.46              |
| 3:N:209:ARG:HH21  | 3:N:391:ALA:CB   | 2.29                     | 0.46              |
| 3:N:603:LEU:O     | 3:N:604:THR:C    | 2.54                     | 0.46              |
| 3:N:615:ARG:HG3   | 3:N:616:GLN:N    | 2.30                     | 0.46              |
| 3:N:671:LYS:C     | 3:N:674:ARG:HB2  | 2.36                     | 0.46              |
| 3:N:853:VAL:O     | 3:N:856:GLY:N    | 2.43                     | 0.46              |
| 4:O:7:ASP:O       | 4:O:10:PHE:HB2   | 2.16                     | 0.46              |
| 5:P:328:PHE:O     | 5:P:329:TYR:C    | 2.54                     | 0.46              |
| 5:P:359:SER:O     | 5:P:361:LEU:N    | 2.49                     | 0.46              |
| 1:A:109:VAL:HB    | 1:A:130:ALA:N    | 2.29                     | 0.46              |
| 1:A:71:VAL:HG22   | 1:A:132:LEU:HD22 | 1.98                     | 0.46              |
| 1:A:65:PHE:CD1    | 1:A:65:PHE:N     | 2.83                     | 0.46              |
| 1:B:195:LEU:HD12  | 1:B:196:THR:H    | 1.81                     | 0.46              |
| 1:B:175:ARG:N     | 1:B:200:TRP:O    | 2.33                     | 0.46              |
| 1:B:41:ARG:NH1    | 1:B:41:ARG:HG3   | 2.31                     | 0.46              |
| 1:B:77:GLU:HB2    | 3:D:872:ARG:NH2  | 2.30                     | 0.46              |
| 2:C:261:ILE:HG22  | 2:C:262:ALA:N    | 2.29                     | 0.46              |
| 2:C:385:PHE:CG    | 2:C:386:PHE:N    | 2.82                     | 0.46              |
| 2:C:400:PRO:O     | 2:C:401:LEU:C    | 2.54                     | 0.46              |
| 2:C:512:ARG:HD3   | 2:C:512:ARG:HA   | 1.82                     | 0.46              |
| 2:C:435:TYR:CE2   | 2:C:516:ARG:CZ   | 2.98                     | 0.46              |
| 2:C:607:ASP:OD1   | 2:C:608:GLY:N    | 2.49                     | 0.46              |
| 2:C:641:PRO:HA    | 2:C:655:LEU:O    | 2.16                     | 0.46              |
| 2:C:630:ARG:NE    | 2:C:705:ILE:O    | 2.48                     | 0.46              |
| 2:C:808:ARG:H     | 2:C:815:LEU:CD1  | 2.29                     | 0.46              |
| 3:D:1124:GLN:HA   | 3:D:1125:PRO:HD3 | 1.64                     | 0.46              |
| 3:D:115:LEU:O     | 3:D:116:LEU:HD23 | 2.16                     | 0.46              |
| 3:D:1292:VAL:O    | 3:D:1303:TYR:N   | 2.44                     | 0.46              |
| 3:D:1360:GLY:HA2  | 3:D:1362:LYS:HZ1 | 1.80                     | 0.46              |
| 3:D:1388:ARG:HG2  | 3:D:1391:GLU:HG3 | 1.97                     | 0.46              |
| 3:D:1462:LEU:HD22 | 3:D:1472:ILE:CD1 | 2.46                     | 0.46              |
| 3:D:1499:ARG:HD3  | 3:D:1499:ARG:C   | 2.36                     | 0.46              |
| 3:D:159:ARG:C     | 3:D:161:LEU:H    | 2.19                     | 0.46              |
| 3:D:178:LEU:CG    | 3:D:181:ASP:HB2  | 2.44                     | 0.46              |
| 3:D:295:GLY:HA3   | 3:D:303:PRO:HD3  | 1.98                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:417:PRO:CB    | 3:D:429:SER:C    | 2.84                     | 0.46              |
| 3:D:60:CYS:SG     | 3:D:62:LYS:HG2   | 2.55                     | 0.46              |
| 3:D:633:VAL:O     | 3:D:635:PRO:HD3  | 2.16                     | 0.46              |
| 2:C:1009:SER:CB   | 3:D:651:GLU:OE2  | 2.63                     | 0.46              |
| 3:D:690:ALA:O     | 3:D:691:LEU:C    | 2.54                     | 0.46              |
| 3:D:858:VAL:CG1   | 3:D:859:ASP:N    | 2.77                     | 0.46              |
| 5:F:296:GLY:HA3   | 5:F:297:PRO:HD2  | 1.53                     | 0.46              |
| 5:F:402:ASN:H     | 5:F:402:ASN:HD22 | 1.61                     | 0.46              |
| 5:F:92:PRO:O      | 5:F:94:LEU:N     | 2.49                     | 0.46              |
| 2:M:135:VAL:HG23  | 2:M:395:LYS:HB2  | 1.96                     | 0.46              |
| 2:M:193:LEU:HD23  | 2:M:307:LEU:HD22 | 1.97                     | 0.46              |
| 2:M:333:ILE:HG21  | 2:M:461:VAL:HG21 | 1.98                     | 0.46              |
| 2:M:479:VAL:HG21  | 2:M:503:LEU:HD21 | 1.97                     | 0.46              |
| 2:M:715:THR:HB    | 2:M:718:GLY:O    | 2.16                     | 0.46              |
| 2:M:536:PRO:HB2   | 2:M:905:ILE:CG2  | 2.46                     | 0.46              |
| 3:N:1108:ARG:HE   | 3:N:1199:GLY:CA  | 2.29                     | 0.46              |
| 3:N:212:ARG:N     | 3:N:386:HIS:O    | 2.40                     | 0.46              |
| 3:N:468:LEU:HD11  | 3:N:473:LEU:HD13 | 1.97                     | 0.46              |
| 3:N:550:ARG:CZ    | 3:N:573:MET:HB3  | 2.44                     | 0.46              |
| 3:N:736:PHE:O     | 3:N:737:ASN:C    | 2.53                     | 0.46              |
| 3:N:704:ARG:NE    | 3:N:738:ALA:HB2  | 2.31                     | 0.46              |
| 3:N:847:ASP:O     | 3:N:848:GLU:C    | 2.54                     | 0.46              |
| 3:N:84:ILE:C      | 3:N:86:ARG:N     | 2.69                     | 0.46              |
| 4:O:57:ASP:O      | 4:O:63:TRP:NE1   | 2.40                     | 0.46              |
| 3:N:545:ARG:HE    | 5:P:257:THR:HA   | 1.81                     | 0.46              |
| 1:B:79:ILE:O      | 1:B:82:LEU:HG    | 2.15                     | 0.46              |
| 1:B:91:ASN:HD22   | 1:B:92:PRO:N     | 2.14                     | 0.46              |
| 2:C:94:LEU:O      | 2:C:114:PHE:HA   | 2.16                     | 0.46              |
| 2:C:341:THR:O     | 2:C:345:ARG:HG3  | 2.16                     | 0.46              |
| 2:C:386:PHE:HD1   | 2:C:386:PHE:H    | 1.64                     | 0.46              |
| 2:C:550:LEU:CD2   | 2:C:905:ILE:HD11 | 2.45                     | 0.46              |
| 2:C:625:LEU:HD12  | 2:C:639:GLN:OE1  | 2.16                     | 0.46              |
| 3:D:1030:GLY:HA2  | 3:D:1034:GLN:NE2 | 2.30                     | 0.46              |
| 3:D:1231:GLU:C    | 3:D:1231:GLU:CD  | 2.75                     | 0.46              |
| 3:D:1283:ILE:HG13 | 3:D:1315:ASP:OD1 | 2.15                     | 0.46              |
| 3:D:135:LEU:HD11  | 3:D:148:GLU:HG3  | 1.98                     | 0.46              |
| 3:D:1388:ARG:N    | 3:D:1391:GLU:OE2 | 2.43                     | 0.46              |
| 3:D:1481:VAL:HG21 | 4:E:18:ARG:HB2   | 1.98                     | 0.46              |
| 3:D:18:ILE:HD12   | 3:D:516:ALA:HB3  | 1.97                     | 0.46              |
| 3:D:262:LYS:HG2   | 3:D:263:GLU:N    | 2.31                     | 0.46              |
| 3:D:575:GLN:OE1   | 3:D:575:GLN:HA   | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:8:VAL:HG12    | 3:D:1434:TRP:CH2  | 2.51                     | 0.46              |
| 3:D:962:GLN:O     | 3:D:965:GLU:N     | 2.48                     | 0.46              |
| 5:F:401:GLU:CG    | 5:F:405:LEU:HD11  | 2.46                     | 0.46              |
| 1:L:70:GLY:HA2    | 1:L:133:GLU:CG    | 2.46                     | 0.46              |
| 2:M:1006:HIS:HA   | 2:M:1027:PHE:CE1  | 2.51                     | 0.46              |
| 2:M:1040:LEU:HD13 | 2:M:1049:LEU:HB2  | 1.97                     | 0.46              |
| 2:M:202:TYR:O     | 2:M:207:LEU:HD11  | 2.16                     | 0.46              |
| 2:M:768:THR:HB    | 2:M:771:GLU:HB3   | 1.98                     | 0.46              |
| 2:M:773:LEU:O     | 2:M:777:ILE:HG13  | 2.16                     | 0.46              |
| 2:M:922:PHE:O     | 2:M:923:GLU:C     | 2.54                     | 0.46              |
| 2:M:930:LYS:O     | 2:M:932:GLU:N     | 2.39                     | 0.46              |
| 2:M:97:ARG:C      | 2:M:98:LEU:HD23   | 2.36                     | 0.46              |
| 3:N:1025:GLN:C    | 3:N:1027:GLY:H    | 2.18                     | 0.46              |
| 3:N:1380:GLU:HB3  | 3:N:1418:LYS:HB3  | 1.96                     | 0.46              |
| 3:N:179:VAL:C     | 3:N:181:ASP:N     | 2.67                     | 0.46              |
| 3:N:182:GLY:HA2   | 3:N:203:ALA:CB    | 2.42                     | 0.46              |
| 3:N:337:LEU:C     | 3:N:338:GLU:HG3   | 2.35                     | 0.46              |
| 3:N:211:VAL:HA    | 3:N:386:HIS:O     | 2.15                     | 0.46              |
| 3:N:441:ARG:C     | 3:N:443:VAL:H     | 2.19                     | 0.46              |
| 3:N:558:LEU:C     | 3:N:560:GLN:H     | 2.17                     | 0.46              |
| 3:N:661:MET:HE2   | 3:N:677:LEU:HD11  | 1.97                     | 0.46              |
| 3:N:855:HIS:O     | 3:N:857:ILE:HG23  | 2.15                     | 0.46              |
| 3:N:881:LEU:O     | 3:N:882:PHE:C     | 2.54                     | 0.46              |
| 4:O:92:ILE:HB     | 4:O:93:TYR:CD1    | 2.51                     | 0.46              |
| 5:P:276:ARG:O     | 5:P:278:LEU:N     | 2.48                     | 0.46              |
| 5:P:385:GLU:HA    | 5:P:388:ALA:CB    | 2.45                     | 0.46              |
| 1:B:91:ASN:HB2    | 1:B:119:ASP:OD2   | 2.15                     | 0.46              |
| 1:B:210:ALA:O     | 1:B:213:GLN:N     | 2.49                     | 0.46              |
| 2:C:1100:GLN:O    | 3:D:9:ARG:N       | 2.39                     | 0.46              |
| 2:C:243:ARG:HG3   | 2:C:244:PRO:CA    | 2.38                     | 0.46              |
| 2:C:335:THR:C     | 2:C:339:LEU:HD12  | 2.36                     | 0.46              |
| 2:C:432:ARG:CG    | 2:C:433:THR:N     | 2.79                     | 0.46              |
| 3:D:1091:SER:O    | 3:D:1093:TYR:N    | 2.49                     | 0.46              |
| 3:D:916:TYR:OH    | 3:D:1168:MET:HB2  | 2.15                     | 0.46              |
| 3:D:775:GLY:HA3   | 3:D:1209:LEU:HD22 | 1.97                     | 0.46              |
| 3:D:1363:LEU:C    | 3:D:1363:LEU:HD23 | 2.36                     | 0.46              |
| 3:D:1383:ASP:CB   | 3:D:1416:ALA:HB3  | 2.46                     | 0.46              |
| 3:D:169:TYR:N     | 3:D:393:ILE:O     | 2.48                     | 0.46              |
| 3:D:14:SER:HB2    | 3:D:17:LYS:CB     | 2.44                     | 0.46              |
| 3:D:256:GLU:HB2   | 3:D:296:GLU:HG2   | 1.98                     | 0.46              |
| 3:D:535:PHE:CD1   | 3:D:535:PHE:N     | 2.84                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:1031:ARG:N   | 3:D:622:ARG:NH1   | 2.63                     | 0.46              |
| 3:D:655:PRO:O    | 3:D:658:LEU:HB2   | 2.16                     | 0.46              |
| 3:D:988:ARG:O    | 3:D:989:TYR:C     | 2.54                     | 0.46              |
| 3:D:990:ASP:O    | 3:D:994:GLN:NE2   | 2.47                     | 0.46              |
| 2:C:1067:TYR:HB2 | 5:F:341:PRO:HB3   | 1.97                     | 0.46              |
| 5:F:392:VAL:CG1  | 5:F:396:ARG:HB3   | 2.46                     | 0.46              |
| 5:F:400:ILE:O    | 5:F:401:GLU:C     | 2.54                     | 0.46              |
| 1:L:110:LYS:HD2  | 1:L:126:ASP:CA    | 2.45                     | 0.46              |
| 1:L:19:GLU:HG2   | 1:L:203:GLY:N     | 2.31                     | 0.46              |
| 1:L:6:LEU:O      | 1:L:8:ALA:N       | 2.45                     | 0.46              |
| 1:L:64:GLU:HA    | 1:L:75:VAL:HG11   | 1.96                     | 0.46              |
| 2:M:1103:ASP:OD1 | 2:M:1105:LYS:HB2  | 2.15                     | 0.46              |
| 2:M:213:ALA:C    | 2:M:215:GLY:N     | 2.68                     | 0.46              |
| 2:M:274:ARG:O    | 2:M:275:TYR:C     | 2.53                     | 0.46              |
| 2:M:693:GLU:HA   | 2:M:696:LYS:HD2   | 1.97                     | 0.46              |
| 2:M:701:THR:OG1  | 2:M:832:LYS:HG3   | 2.16                     | 0.46              |
| 2:M:833:LEU:HD12 | 2:M:837:ASP:CG    | 2.35                     | 0.46              |
| 3:N:1094:LEU:O   | 3:N:1097:LYS:N    | 2.48                     | 0.46              |
| 3:N:1232:PRO:O   | 3:N:1235:GLN:HG2  | 2.16                     | 0.46              |
| 3:N:1404:ASN:OD1 | 3:N:1408:ILE:HG22 | 2.15                     | 0.46              |
| 3:N:1103:HIS:CD2 | 3:N:1463:LYS:H    | 2.34                     | 0.46              |
| 3:N:259:VAL:HG23 | 3:N:270:LEU:CD1   | 2.44                     | 0.46              |
| 3:N:372:ASP:C    | 3:N:374:GLU:H     | 2.19                     | 0.46              |
| 3:N:566:ILE:C    | 3:N:569:ASN:HB3   | 2.35                     | 0.46              |
| 3:N:630:VAL:HA   | 3:N:744:GLN:HA    | 1.98                     | 0.46              |
| 3:N:846:PRO:O    | 3:N:847:ASP:C     | 2.53                     | 0.46              |
| 4:O:48:MET:O     | 4:O:54:LEU:HA     | 2.16                     | 0.46              |
| 5:P:401:GLU:O    | 5:P:402:ASN:C     | 2.54                     | 0.46              |
| 1:B:206:THR:O    | 1:B:207:PRO:C     | 2.54                     | 0.46              |
| 1:B:208:LEU:O    | 1:B:209:GLU:C     | 2.54                     | 0.46              |
| 2:C:191:PHE:CD2  | 2:C:195:LEU:HD11  | 2.49                     | 0.46              |
| 2:C:219:GLN:C    | 2:C:221:LEU:N     | 2.65                     | 0.46              |
| 2:C:275:TYR:CE1  | 2:C:279:GLU:OE1   | 2.69                     | 0.46              |
| 2:C:3:ILE:HD11   | 2:C:5:ARG:HE      | 1.80                     | 0.46              |
| 2:C:717:LEU:HD21 | 2:C:764:GLU:HG3   | 1.97                     | 0.46              |
| 2:C:712:ALA:C    | 2:C:820:ARG:HG3   | 2.36                     | 0.46              |
| 3:D:113:GLY:O    | 3:D:115:LEU:N     | 2.49                     | 0.46              |
| 3:D:1153:VAL:O   | 3:D:1159:ARG:HA   | 2.15                     | 0.46              |
| 3:D:1260:ILE:O   | 3:D:1261:GLU:C    | 2.54                     | 0.46              |
| 3:D:42:ASP:OD1   | 3:D:48:ARG:NH2    | 2.49                     | 0.46              |
| 3:D:522:PRO:CA   | 3:D:525:ARG:NH1   | 2.79                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:548:ILE:O    | 3:D:549:ASN:C    | 2.54                     | 0.46              |
| 3:D:59:ALA:C     | 3:D:61:GLY:N     | 2.70                     | 0.46              |
| 3:D:695:ILE:O    | 3:D:696:HIS:C    | 2.54                     | 0.46              |
| 3:D:709:HIS:O    | 3:D:710:ARG:C    | 2.54                     | 0.46              |
| 3:D:96:ALA:HB3   | 3:D:554:LEU:CD2  | 2.46                     | 0.46              |
| 5:F:406:ARG:HA   | 5:F:409:LYS:HE3  | 1.98                     | 0.46              |
| 1:K:108:GLU:HG3  | 1:K:131:THR:HG22 | 1.96                     | 0.46              |
| 2:M:313:LEU:O    | 2:M:315:ALA:N    | 2.49                     | 0.46              |
| 2:M:352:ALA:O    | 2:M:356:ARG:HG3  | 2.16                     | 0.46              |
| 2:M:401:LEU:O    | 2:M:402:SER:C    | 2.54                     | 0.46              |
| 2:M:645:VAL:C    | 2:M:647:GLN:H    | 2.19                     | 0.46              |
| 2:M:682:TYR:C    | 2:M:684:PHE:H    | 2.19                     | 0.46              |
| 2:M:790:LEU:HD12 | 2:M:791:ARG:N    | 2.30                     | 0.46              |
| 3:N:104:PHE:O    | 3:N:112:ILE:HD11 | 2.16                     | 0.46              |
| 3:N:1348:LEU:O   | 3:N:1349:VAL:C   | 2.53                     | 0.46              |
| 3:N:259:VAL:HG22 | 3:N:260:GLU:N    | 2.31                     | 0.46              |
| 3:N:471:GLU:O    | 3:N:474:GLU:HB3  | 2.15                     | 0.46              |
| 3:N:630:VAL:HG22 | 3:N:744:GLN:CG   | 2.46                     | 0.46              |
| 3:N:660:LYS:CG   | 3:N:694:VAL:HG22 | 2.46                     | 0.46              |
| 3:N:990:ASP:HA   | 3:N:993:LEU:CG   | 2.46                     | 0.46              |
| 5:P:102:LEU:HD11 | 5:P:183:ALA:C    | 2.36                     | 0.46              |
| 5:P:207:LEU:HB3  | 5:P:212:LEU:CD2  | 2.46                     | 0.46              |
| 5:P:382:THR:O    | 5:P:386:VAL:HG13 | 2.16                     | 0.46              |
| 2:C:1089:VAL:O   | 2:C:1092:LEU:HB2 | 2.15                     | 0.45              |
| 2:C:192:PRO:O    | 2:C:195:LEU:CG   | 2.61                     | 0.45              |
| 2:C:285:LEU:HD11 | 2:C:288:ARG:O    | 2.15                     | 0.45              |
| 2:C:323:ASP:O    | 2:C:325:ILE:HD12 | 2.15                     | 0.45              |
| 2:C:383:ARG:O    | 2:C:387:SER:OG   | 2.32                     | 0.45              |
| 2:C:499:ALA:HA   | 2:C:532:MET:HG2  | 1.98                     | 0.45              |
| 2:C:577:PRO:HG3  | 2:C:993:PHE:CD2  | 2.51                     | 0.45              |
| 2:C:754:ILE:HG12 | 2:C:791:ARG:HD3  | 1.97                     | 0.45              |
| 2:C:943:VAL:O    | 2:C:946:ARG:HB3  | 2.17                     | 0.45              |
| 3:D:259:VAL:HG21 | 3:D:292:VAL:C    | 2.35                     | 0.45              |
| 3:D:302:GLN:O    | 3:D:304:LEU:HG   | 2.16                     | 0.45              |
| 3:D:685:ASP:C    | 3:D:687:VAL:N    | 2.69                     | 0.45              |
| 3:D:885:ILE:O    | 3:D:888:GLU:HB2  | 2.16                     | 0.45              |
| 4:E:92:ILE:HG13  | 4:E:92:ILE:H     | 1.57                     | 0.45              |
| 5:F:110:MET:HE3  | 5:F:111:GLU:HG3  | 1.98                     | 0.45              |
| 5:F:140:ARG:O    | 5:F:140:ARG:HG2  | 2.16                     | 0.45              |
| 5:F:168:LYS:O    | 5:F:172:ARG:N    | 2.42                     | 0.45              |
| 5:F:174:LEU:HD12 | 5:F:174:LEU:C    | 2.37                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:238:TYR:CD2  | 5:F:239:ALA:N    | 2.84                     | 0.45              |
| 1:K:186:LEU:HD23 | 1:K:188:GLN:HE21 | 1.81                     | 0.45              |
| 1:L:44:LEU:O     | 1:L:174:VAL:HG21 | 2.16                     | 0.45              |
| 2:M:261:ILE:O    | 2:M:264:PRO:HD2  | 2.16                     | 0.45              |
| 2:M:350:ARG:HA   | 2:M:353:ARG:CD   | 2.46                     | 0.45              |
| 2:M:512:ARG:HB3  | 2:M:523:ILE:HG13 | 1.98                     | 0.45              |
| 1:K:69:PRO:HA    | 2:M:607:ASP:OD1  | 2.16                     | 0.45              |
| 3:N:1282:ARG:NH2 | 3:N:1293:PHE:CD2 | 2.84                     | 0.45              |
| 3:N:274:ARG:CD   | 3:N:279:VAL:HG11 | 2.46                     | 0.45              |
| 3:N:162:ARG:NH1  | 3:N:434:ARG:HH22 | 2.14                     | 0.45              |
| 3:N:56:TYR:CE2   | 3:N:66:GLN:HG3   | 2.51                     | 0.45              |
| 3:N:887:ALA:CA   | 3:N:890:VAL:HG22 | 2.46                     | 0.45              |
| 3:N:989:TYR:CE2  | 3:N:993:LEU:HD11 | 2.51                     | 0.45              |
| 4:O:55:PHE:N     | 4:O:55:PHE:CD1   | 2.84                     | 0.45              |
| 5:P:382:THR:HG22 | 5:P:394:ARG:CA   | 2.46                     | 0.45              |
| 5:P:403:LYS:HD2  | 5:P:407:LYS:HE2  | 1.97                     | 0.45              |
| 5:P:412:GLU:C    | 5:P:414:ARG:H    | 2.18                     | 0.45              |
| 1:A:159:LYS:NZ   | 1:A:164:ALA:O    | 2.40                     | 0.45              |
| 2:C:1014:SER:N   | 2:C:1021:LEU:HB2 | 2.32                     | 0.45              |
| 2:C:243:ARG:CG   | 2:C:244:PRO:CA   | 2.92                     | 0.45              |
| 2:C:395:LYS:CE   | 2:C:403:SER:HB2  | 2.44                     | 0.45              |
| 2:C:543:ASN:HA   | 2:C:546:LEU:HD12 | 1.98                     | 0.45              |
| 2:C:645:VAL:C    | 2:C:647:GLN:H    | 2.18                     | 0.45              |
| 2:C:799:ILE:O    | 2:C:801:VAL:HG13 | 2.17                     | 0.45              |
| 2:C:903:SER:OG   | 2:C:908:GLY:HA3  | 2.16                     | 0.45              |
| 2:C:910:LYS:CG   | 2:C:912:PRO:HD2  | 2.29                     | 0.45              |
| 2:C:976:ASP:OD2  | 2:C:979:THR:HG23 | 2.16                     | 0.45              |
| 3:D:1173:LEU:O   | 3:D:1176:LYS:N   | 2.49                     | 0.45              |
| 3:D:1380:GLU:N   | 3:D:1420:LEU:HG  | 2.31                     | 0.45              |
| 3:D:493:ARG:HB2  | 3:D:1388:ARG:HD2 | 1.97                     | 0.45              |
| 3:D:355:VAL:CG1  | 3:D:356:PRO:HD2  | 2.46                     | 0.45              |
| 3:D:520:LEU:CG   | 3:D:524:LEU:HB2  | 2.46                     | 0.45              |
| 3:D:699:VAL:CG1  | 3:D:717:GLN:HG2  | 2.42                     | 0.45              |
| 3:D:646:LYS:HG2  | 3:D:720:LEU:HB3  | 1.98                     | 0.45              |
| 3:D:808:THR:OG1  | 3:D:809:PRO:HD3  | 2.17                     | 0.45              |
| 3:D:828:LYS:CD   | 3:D:828:LYS:N    | 2.79                     | 0.45              |
| 3:D:884:ARG:C    | 3:D:888:GLU:HG2  | 2.36                     | 0.45              |
| 5:F:123:ASP:HB2  | 5:F:126:LEU:HB2  | 1.98                     | 0.45              |
| 5:F:134:LYS:HB3  | 5:F:178:ARG:HH12 | 1.81                     | 0.45              |
| 5:F:209:PHE:CA   | 5:F:212:LEU:HG   | 2.46                     | 0.45              |
| 5:F:214:GLN:HA   | 5:F:217:ASN:ND2  | 2.11                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:287:THR:OG1  | 5:F:288:TYR:N    | 2.48                     | 0.45              |
| 2:M:23:VAL:HG12  | 2:M:121:MET:CE   | 2.46                     | 0.45              |
| 2:M:32:ALA:C     | 2:M:35:PRO:HD2   | 2.36                     | 0.45              |
| 2:M:41:ASN:ND2   | 2:M:42:VAL:N     | 2.64                     | 0.45              |
| 2:M:615:TYR:O    | 2:M:616:GLU:C    | 2.55                     | 0.45              |
| 2:M:627:ARG:O    | 2:M:629:TYR:CD1  | 2.70                     | 0.45              |
| 2:M:397:GLU:CG   | 2:M:632:ASN:HB2  | 2.43                     | 0.45              |
| 2:M:728:HIS:CD2  | 2:M:730:SER:O    | 2.69                     | 0.45              |
| 2:M:918:LEU:HD12 | 2:M:968:LEU:CA   | 2.44                     | 0.45              |
| 3:N:1018:ASN:OD1 | 3:N:1020:LEU:N   | 2.49                     | 0.45              |
| 3:N:1336:LEU:HB3 | 3:N:1337:GLU:OE1 | 2.16                     | 0.45              |
| 3:N:152:LEU:CG   | 3:N:153:LEU:N    | 2.79                     | 0.45              |
| 3:N:154:THR:HG22 | 3:N:157:GLU:HB2  | 1.97                     | 0.45              |
| 3:N:372:ASP:OD2  | 3:N:374:GLU:O    | 2.34                     | 0.45              |
| 3:N:839:LEU:O    | 3:N:840:LYS:C    | 2.54                     | 0.45              |
| 4:O:88:GLU:HA    | 4:O:91:ARG:HD2   | 1.99                     | 0.45              |
| 5:P:209:PHE:CA   | 5:P:212:LEU:HG   | 2.47                     | 0.45              |
| 3:N:674:ARG:NH2  | 5:P:342:VAL:HG13 | 2.31                     | 0.45              |
| 1:A:51:THR:HA    | 1:A:145:ASP:O    | 2.17                     | 0.45              |
| 1:A:181:VAL:CG1  | 1:A:193:ASP:HB3  | 2.46                     | 0.45              |
| 1:A:206:THR:HG21 | 1:A:208:LEU:HB3  | 1.96                     | 0.45              |
| 1:A:7:LYS:HA     | 1:A:7:LYS:HD3    | 1.66                     | 0.45              |
| 1:B:176:ARG:HD2  | 1:B:200:TRP:NE1  | 2.32                     | 0.45              |
| 1:B:26:GLU:HB2   | 1:B:27:PRO:HA    | 1.98                     | 0.45              |
| 2:C:1082:PRO:O   | 2:C:1083:GLU:C   | 2.53                     | 0.45              |
| 2:C:12:VAL:HG23  | 2:C:13:ILE:CD1   | 2.46                     | 0.45              |
| 2:C:441:VAL:CG1  | 2:C:544:THR:HG21 | 2.46                     | 0.45              |
| 2:C:441:VAL:HG11 | 2:C:544:THR:HG21 | 1.98                     | 0.45              |
| 2:C:462:ASP:O    | 2:C:465:GLY:N    | 2.42                     | 0.45              |
| 2:C:503:LEU:HD11 | 2:C:506:ASN:O    | 2.16                     | 0.45              |
| 2:C:728:HIS:CE1  | 2:C:730:SER:N    | 2.85                     | 0.45              |
| 2:C:854:PRO:O    | 2:C:856:GLU:N    | 2.49                     | 0.45              |
| 2:C:839:LEU:CD2  | 2:C:996:LYS:HA   | 2.45                     | 0.45              |
| 3:D:127:LEU:HA   | 3:D:132:TYR:O    | 2.16                     | 0.45              |
| 3:D:1379:VAL:HA  | 3:D:1420:LEU:HG  | 1.98                     | 0.45              |
| 3:D:185:VAL:HG23 | 3:D:203:ALA:N    | 2.30                     | 0.45              |
| 3:D:540:LEU:O    | 3:D:543:LEU:N    | 2.49                     | 0.45              |
| 3:D:823:LEU:O    | 3:D:823:LEU:HG   | 2.16                     | 0.45              |
| 3:D:884:ARG:O    | 3:D:886:VAL:N    | 2.50                     | 0.45              |
| 3:D:770:LEU:HD11 | 3:D:919:PHE:CE1  | 2.52                     | 0.45              |
| 3:D:959:GLU:HB3  | 3:D:963:TYR:CZ   | 2.50                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:410:TYR:HA    | 5:F:413:SER:OG    | 2.15                     | 0.45              |
| 1:K:186:LEU:N     | 1:K:189:ARG:O     | 2.49                     | 0.45              |
| 1:K:68:ILE:CG2    | 1:K:69:PRO:HD2    | 2.43                     | 0.45              |
| 2:M:1017:THR:O    | 2:M:1018:GLN:HB2  | 2.15                     | 0.45              |
| 2:M:267:TYR:CE2   | 2:M:271:GLU:HB2   | 2.51                     | 0.45              |
| 2:M:274:ARG:HH21  | 2:M:284:ARG:CD    | 2.29                     | 0.45              |
| 2:M:57:GLU:HG3    | 2:M:62:GLY:O      | 2.16                     | 0.45              |
| 2:M:603:VAL:HG12  | 2:M:645:VAL:HA    | 1.96                     | 0.45              |
| 2:M:88:LEU:O      | 2:M:131:GLY:N     | 2.34                     | 0.45              |
| 3:N:1127:GLU:OE2  | 3:N:1133:ARG:HD2  | 2.17                     | 0.45              |
| 3:N:1468:LEU:CD2  | 3:N:1468:LEU:C    | 2.85                     | 0.45              |
| 3:N:1468:LEU:HD22 | 3:N:1470:ARG:N    | 2.31                     | 0.45              |
| 3:N:297:ILE:HB    | 3:N:302:GLN:NE2   | 2.32                     | 0.45              |
| 3:N:465:LEU:HD22  | 3:N:509:PRO:HB2   | 1.98                     | 0.45              |
| 3:N:731:LEU:CD1   | 3:N:931:LEU:HB3   | 2.47                     | 0.45              |
| 4:O:64:ALA:O      | 4:O:65:MET:C      | 2.55                     | 0.45              |
| 5:P:231:ARG:HB3   | 5:P:233:PHE:CE2   | 2.51                     | 0.45              |
| 5:P:271:LEU:H     | 5:P:271:LEU:HD23  | 1.80                     | 0.45              |
| 5:P:364:ARG:HB3   | 5:P:389:PHE:HZ    | 1.81                     | 0.45              |
| 1:A:143:ARG:HH11  | 1:A:158:ILE:HG23  | 1.82                     | 0.45              |
| 1:A:41:ARG:CG     | 1:A:45:LEU:HD11   | 2.46                     | 0.45              |
| 1:A:54:THR:CG2    | 1:A:158:ILE:HG13  | 2.46                     | 0.45              |
| 1:B:10:VAL:N      | 1:B:26:GLU:O      | 2.43                     | 0.45              |
| 1:B:41:ARG:CA     | 1:B:44:LEU:HD12   | 2.35                     | 0.45              |
| 2:C:135:VAL:HG23  | 2:C:395:LYS:CA    | 2.44                     | 0.45              |
| 2:C:34:VAL:O      | 2:C:36:PRO:HD3    | 2.17                     | 0.45              |
| 2:C:376:ARG:N     | 2:C:377:PRO:HD2   | 2.31                     | 0.45              |
| 2:C:471:TYR:HB3   | 2:C:531:PHE:CD2   | 2.50                     | 0.45              |
| 2:C:643:VAL:HG22  | 2:C:644:VAL:N     | 2.31                     | 0.45              |
| 2:C:87:ASP:CG     | 2:C:824:ARG:HH22  | 2.20                     | 0.45              |
| 3:D:1081:GLY:O    | 3:D:1084:THR:HG23 | 2.15                     | 0.45              |
| 3:D:1088:THR:HG23 | 3:D:1089:ALA:N    | 2.31                     | 0.45              |
| 3:D:1342:GLU:N    | 3:D:1342:GLU:CD   | 2.69                     | 0.45              |
| 3:D:1342:GLU:OE1  | 3:D:1342:GLU:N    | 2.40                     | 0.45              |
| 3:D:227:LEU:CD2   | 3:D:326:GLU:OE2   | 2.65                     | 0.45              |
| 3:D:550:ARG:HH11  | 3:D:573:MET:C     | 2.20                     | 0.45              |
| 3:D:766:ALA:O     | 3:D:767:HIS:HD2   | 1.99                     | 0.45              |
| 3:D:843:PHE:HB2   | 3:D:866:VAL:HG22  | 1.97                     | 0.45              |
| 3:D:862:ASP:O     | 3:D:876:SER:HB2   | 2.16                     | 0.45              |
| 3:D:970:LYS:HA    | 3:D:973:GLN:HE21  | 1.81                     | 0.45              |
| 4:E:10:PHE:O      | 4:E:12:MET:N      | 2.50                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:206:GLY:O    | 5:F:207:LEU:HB2   | 2.16                     | 0.45              |
| 5:F:285:GLU:OE1  | 5:F:285:GLU:HA    | 2.15                     | 0.45              |
| 1:L:30:ARG:HD3   | 2:M:854:PRO:HB3   | 1.98                     | 0.45              |
| 1:L:38:ASN:O     | 1:L:42:ARG:HG3    | 2.15                     | 0.45              |
| 2:M:1090:LYS:O   | 2:M:1093:GLN:HB2  | 2.17                     | 0.45              |
| 2:M:198:ARG:NE   | 2:M:231:PRO:HD3   | 2.30                     | 0.45              |
| 2:M:241:LEU:N    | 2:M:241:LEU:HD23  | 2.32                     | 0.45              |
| 2:M:31:GLN:O     | 2:M:35:PRO:HB2    | 2.17                     | 0.45              |
| 2:M:408:ARG:NH2  | 2:M:457:ALA:O     | 2.49                     | 0.45              |
| 2:M:600:ASP:CA   | 2:M:650:ARG:HA    | 2.46                     | 0.45              |
| 2:M:681:GLY:O    | 2:M:684:PHE:HB2   | 2.16                     | 0.45              |
| 2:M:774:LEU:HA   | 2:M:777:ILE:CD1   | 2.40                     | 0.45              |
| 3:N:614:PHE:CZ   | 10:N:1528:NE6:H23 | 2.51                     | 0.45              |
| 3:N:373:PRO:O    | 3:N:376:GLU:OE1   | 2.35                     | 0.45              |
| 3:N:460:ALA:O    | 3:N:463:GLN:HB2   | 2.16                     | 0.45              |
| 3:N:709:HIS:NE2  | 3:N:711:LEU:HB2   | 2.32                     | 0.45              |
| 3:N:84:ILE:O     | 3:N:86:ARG:N      | 2.49                     | 0.45              |
| 3:N:879:ARG:HB3  | 3:N:902:LEU:CD1   | 2.46                     | 0.45              |
| 4:O:40:LEU:HD12  | 4:O:41:GLU:HG2    | 1.97                     | 0.45              |
| 5:P:251:ILE:O    | 5:P:255:ALA:CB    | 2.64                     | 0.45              |
| 5:P:393:THR:HG22 | 5:P:395:GLU:H     | 1.81                     | 0.45              |
| 1:A:112:ARG:HE   | 1:A:125:PRO:HB2   | 1.81                     | 0.45              |
| 1:B:56:VAL:HG13  | 1:B:142:VAL:HA    | 1.99                     | 0.45              |
| 2:C:151:ASP:CB   | 2:C:158:TYR:HA    | 2.47                     | 0.45              |
| 2:C:187:ASN:C    | 2:C:188:LYS:HG2   | 2.36                     | 0.45              |
| 2:C:205:GLU:HA   | 2:C:209:ARG:HH11  | 1.82                     | 0.45              |
| 2:C:227:PHE:H    | 2:C:227:PHE:HD1   | 1.65                     | 0.45              |
| 2:C:20:GLU:HA    | 2:C:23:VAL:CG2    | 2.47                     | 0.45              |
| 2:C:275:TYR:O    | 2:C:279:GLU:HB3   | 2.17                     | 0.45              |
| 2:C:36:PRO:HG2   | 2:C:38:LYS:CG     | 2.47                     | 0.45              |
| 2:C:385:PHE:O    | 2:C:386:PHE:C     | 2.54                     | 0.45              |
| 2:C:399:ASN:CB   | 2:C:400:PRO:CD    | 2.95                     | 0.45              |
| 2:C:577:PRO:HG3  | 2:C:993:PHE:CD1   | 2.52                     | 0.45              |
| 2:C:604:ALA:HB3  | 2:C:612:VAL:O     | 2.16                     | 0.45              |
| 2:C:63:GLY:O     | 2:C:102:HIS:HA    | 2.17                     | 0.45              |
| 2:C:714:ASP:OD2  | 2:C:820:ARG:NE    | 2.50                     | 0.45              |
| 2:C:691:SER:HB3  | 2:C:868:ASP:HA    | 1.97                     | 0.45              |
| 2:C:910:LYS:HE3  | 2:C:912:PRO:CG    | 2.46                     | 0.45              |
| 2:C:986:PRO:O    | 2:C:987:ILE:HD13  | 2.17                     | 0.45              |
| 3:D:1103:HIS:CD2 | 3:D:1463:LYS:N    | 2.79                     | 0.45              |
| 3:D:1105:ILE:HA  | 3:D:1198:TYR:O    | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:1211:MET:CB  | 3:D:1213:ARG:NH1 | 2.79                     | 0.45              |
| 3:D:1479:ASP:HA  | 3:D:1482:ARG:CG  | 2.46                     | 0.45              |
| 3:D:274:ARG:HE   | 3:D:279:VAL:HG21 | 1.82                     | 0.45              |
| 3:D:463:GLN:HA   | 3:D:463:GLN:NE2  | 2.32                     | 0.45              |
| 2:C:1094:ALA:HA  | 3:D:518:PRO:HB2  | 1.98                     | 0.45              |
| 3:D:575:GLN:CA   | 3:D:575:GLN:OE1  | 2.65                     | 0.45              |
| 3:D:584:ASN:H    | 3:D:602:SER:CB   | 2.29                     | 0.45              |
| 3:D:966:GLU:HA   | 3:D:969:ARG:NH2  | 2.31                     | 0.45              |
| 5:F:256:ARG:HG2  | 5:F:258:ILE:H    | 1.81                     | 0.45              |
| 1:K:189:ARG:HB2  | 1:K:192:LEU:HD11 | 1.98                     | 0.45              |
| 1:K:183:ASP:OD1  | 1:K:190:THR:O    | 2.33                     | 0.45              |
| 1:K:58:ILE:O     | 1:K:59:GLU:C     | 2.55                     | 0.45              |
| 2:M:235:LEU:HD22 | 2:M:236:ILE:CG1  | 2.47                     | 0.45              |
| 2:M:479:VAL:HB   | 2:M:506:ASN:OD1  | 2.16                     | 0.45              |
| 2:M:546:LEU:C    | 2:M:581:THR:HG21 | 2.37                     | 0.45              |
| 2:M:607:ASP:O    | 2:M:609:ASN:N    | 2.50                     | 0.45              |
| 2:M:712:ALA:CB   | 2:M:821:GLU:HG2  | 2.46                     | 0.45              |
| 2:M:728:HIS:NE2  | 2:M:733:ALA:HB3  | 2.32                     | 0.45              |
| 2:M:73:LEU:C     | 2:M:73:LEU:HD12  | 2.37                     | 0.45              |
| 2:M:961:GLU:O    | 2:M:962:GLN:C    | 2.54                     | 0.45              |
| 3:N:1034:GLN:O   | 3:N:1037:GLN:HB2 | 2.17                     | 0.45              |
| 3:N:1048:PRO:CG  | 3:N:1075:HIS:CD2 | 2.95                     | 0.45              |
| 3:N:1194:CYS:HA  | 3:N:1204:CYS:SG  | 2.56                     | 0.45              |
| 3:N:215:TYR:HD1  | 3:N:381:ALA:O    | 1.99                     | 0.45              |
| 3:N:438:ASP:O    | 3:N:439:LEU:HD23 | 2.16                     | 0.45              |
| 3:N:491:LYS:O    | 3:N:492:ALA:C    | 2.55                     | 0.45              |
| 4:O:40:LEU:HD21  | 4:O:44:GLU:CB    | 2.47                     | 0.45              |
| 5:P:132:ARG:O    | 5:P:133:ALA:C    | 2.55                     | 0.45              |
| 5:P:261:PRO:C    | 5:P:264:MET:HB2  | 2.37                     | 0.45              |
| 5:P:306:GLU:O    | 5:P:310:ILE:HG13 | 2.16                     | 0.45              |
| 5:P:402:ASN:O    | 5:P:406:ARG:HG3  | 2.16                     | 0.45              |
| 1:A:105:GLY:O    | 1:A:107:LYS:HG2  | 2.16                     | 0.45              |
| 1:A:219:ARG:O    | 1:A:220:GLU:C    | 2.54                     | 0.45              |
| 1:A:29:GLU:O     | 1:A:30:ARG:C     | 2.54                     | 0.45              |
| 1:B:212:ASN:N    | 1:B:212:ASN:OD1  | 2.47                     | 0.45              |
| 1:B:40:LEU:O     | 1:B:41:ARG:C     | 2.54                     | 0.45              |
| 2:C:175:GLU:O    | 2:C:176:VAL:CG1  | 2.59                     | 0.45              |
| 2:C:432:ARG:NH1  | 2:C:518:LYS:O    | 2.50                     | 0.45              |
| 2:C:54:ILE:HG23  | 2:C:54:ILE:O     | 2.16                     | 0.45              |
| 2:C:771:GLU:O    | 2:C:772:ARG:C    | 2.54                     | 0.45              |
| 3:D:109:PRO:O    | 3:D:111:LYS:N    | 2.49                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:1396:GLU:O   | 3:D:1397:LYS:CD  | 2.65                     | 0.45              |
| 3:D:441:ARG:CB   | 3:D:443:VAL:HG23 | 2.47                     | 0.45              |
| 3:D:569:ASN:HD21 | 5:F:214:GLN:NE2  | 2.15                     | 0.45              |
| 3:D:773:ALA:HA   | 3:D:1367:HIS:NE2 | 2.31                     | 0.45              |
| 5:F:110:MET:HE3  | 5:F:111:GLU:N    | 2.32                     | 0.45              |
| 5:F:157:GLU:HB3  | 5:F:161:GLN:OE1  | 2.16                     | 0.45              |
| 5:F:220:LEU:O    | 5:F:223:ALA:HB3  | 2.17                     | 0.45              |
| 5:F:321:ILE:HD11 | 5:F:329:TYR:CA   | 2.47                     | 0.45              |
| 5:F:84:TYR:O     | 5:F:87:GLU:HG2   | 2.17                     | 0.45              |
| 1:K:143:ARG:HH11 | 1:K:158:ILE:CG2  | 2.29                     | 0.45              |
| 1:K:18:ARG:O     | 1:K:207:PRO:HD3  | 2.15                     | 0.45              |
| 1:K:215:VAL:O    | 1:K:218:LEU:HB3  | 2.15                     | 0.45              |
| 1:L:120:VAL:HG12 | 1:L:121:GLU:N    | 2.31                     | 0.45              |
| 1:L:28:LEU:HD22  | 1:L:29:GLU:N     | 2.32                     | 0.45              |
| 1:L:28:LEU:HD22  | 1:L:29:GLU:H     | 1.81                     | 0.45              |
| 2:M:148:PHE:CZ   | 2:M:309:TYR:HD2  | 2.35                     | 0.45              |
| 2:M:199:VAL:HG21 | 2:M:238:LEU:HD12 | 1.96                     | 0.45              |
| 2:M:138:SER:HB2  | 2:M:333:ILE:HD11 | 1.98                     | 0.45              |
| 2:M:335:THR:O    | 2:M:339:LEU:HG   | 2.16                     | 0.45              |
| 2:M:672:VAL:HG23 | 2:M:673:LEU:H    | 1.81                     | 0.45              |
| 2:M:833:LEU:HD12 | 2:M:837:ASP:OD2  | 2.17                     | 0.45              |
| 2:M:889:HIS:CE1  | 2:M:970:GLY:HA3  | 2.52                     | 0.45              |
| 3:N:1334:GLN:O   | 3:N:1337:GLU:HB2 | 2.17                     | 0.45              |
| 3:N:1339:LYS:HB3 | 3:N:1343:ALA:CB  | 2.47                     | 0.45              |
| 3:N:1364:HIS:ND1 | 3:N:1365:ASP:N   | 2.64                     | 0.45              |
| 3:N:153:LEU:HG   | 3:N:154:THR:N    | 2.31                     | 0.45              |
| 3:N:320:ALA:O    | 3:N:335:LEU:HB3  | 2.16                     | 0.45              |
| 3:N:3:LYS:HE2    | 3:N:3:LYS:HB3    | 1.77                     | 0.45              |
| 3:N:438:ASP:HA   | 3:N:445:ARG:HH22 | 1.82                     | 0.45              |
| 3:N:462:GLN:HB2  | 3:N:513:ILE:HG12 | 1.99                     | 0.45              |
| 3:N:570:GLU:HB2  | 5:P:214:GLN:HE21 | 1.81                     | 0.45              |
| 3:N:993:LEU:O    | 3:N:994:GLN:C    | 2.54                     | 0.45              |
| 3:N:996:TRP:O    | 3:N:997:THR:C    | 2.55                     | 0.45              |
| 5:P:361:LEU:CG   | 5:P:362:SER:N    | 2.80                     | 0.45              |
| 5:P:367:MET:HB2  | 5:P:371:LEU:HD11 | 1.98                     | 0.45              |
| 5:P:386:VAL:HG11 | 5:P:394:ARG:H    | 1.82                     | 0.45              |
| 2:C:162:ILE:HB   | 2:C:172:ILE:HB   | 1.98                     | 0.45              |
| 2:C:257:VAL:O    | 2:C:261:ILE:HB   | 2.17                     | 0.45              |
| 2:C:268:ASP:OD2  | 2:C:268:ASP:N    | 2.50                     | 0.45              |
| 2:C:499:ALA:O    | 2:C:501:THR:N    | 2.50                     | 0.45              |
| 2:C:578:VAL:CG2  | 2:C:579:VAL:HG12 | 2.44                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:583:LEU:O     | 2:C:587:VAL:HG23  | 2.17                     | 0.45              |
| 2:C:596:TYR:CD1   | 2:C:596:TYR:N     | 2.84                     | 0.45              |
| 2:C:674:VAL:HG21  | 2:C:871:LEU:CD1   | 2.45                     | 0.45              |
| 2:C:910:LYS:HG2   | 2:C:913:GLU:CD    | 2.37                     | 0.45              |
| 2:C:674:VAL:HG11  | 2:C:992:MET:CB    | 2.46                     | 0.45              |
| 3:D:1197:ARG:HG2  | 3:D:1198:TYR:CE2  | 2.52                     | 0.45              |
| 3:D:1323:GLN:HG3  | 3:D:1324:PRO:HD2  | 1.98                     | 0.45              |
| 3:D:1436:SER:O    | 3:D:1439:SER:N    | 2.49                     | 0.45              |
| 3:D:1486:VAL:HG22 | 4:E:75:PHE:CA     | 2.45                     | 0.45              |
| 3:D:460:ALA:O     | 3:D:463:GLN:HB2   | 2.17                     | 0.45              |
| 3:D:531:ASP:O     | 3:D:532:GLY:C     | 2.55                     | 0.45              |
| 3:D:567:ILE:CD1   | 5:F:140:ARG:HH22  | 2.29                     | 0.45              |
| 3:D:57:GLU:CG     | 3:D:64:LYS:HA     | 2.38                     | 0.45              |
| 3:D:812:ALA:HA    | 3:D:816:HIS:CB    | 2.26                     | 0.45              |
| 5:F:175:HIS:C     | 5:F:178:ARG:HB2   | 2.37                     | 0.45              |
| 3:D:65:ARG:CB     | 5:F:375:LEU:O     | 2.64                     | 0.45              |
| 1:K:74:ASP:C      | 1:K:74:ASP:OD1    | 2.55                     | 0.45              |
| 2:M:1091:GLU:O    | 2:M:1095:LEU:HG   | 2.17                     | 0.45              |
| 2:M:1111:ILE:HG13 | 2:M:1112:PHE:CD1  | 2.52                     | 0.45              |
| 2:M:23:VAL:CA     | 2:M:121:MET:HE1   | 2.42                     | 0.45              |
| 2:M:164:PRO:HA    | 2:M:266:ARG:HA    | 1.98                     | 0.45              |
| 2:M:395:LYS:HE2   | 2:M:403:SER:HB3   | 1.99                     | 0.45              |
| 2:M:439:CYS:HB2   | 2:M:541:SER:N     | 2.32                     | 0.45              |
| 2:M:446:GLY:O     | 2:M:448:ASN:N     | 2.50                     | 0.45              |
| 2:M:446:GLY:O     | 2:M:449:ILE:N     | 2.47                     | 0.45              |
| 2:M:469:THR:HG22  | 2:M:470:PRO:O     | 2.16                     | 0.45              |
| 2:M:726:ILE:CG1   | 2:M:728:HIS:HB2   | 2.47                     | 0.45              |
| 2:M:945:ARG:O     | 2:M:948:GLU:HG2   | 2.17                     | 0.45              |
| 2:M:99:GLN:HA     | 2:M:109:LYS:HA    | 1.98                     | 0.45              |
| 3:N:1020:LEU:O    | 3:N:1021:TYR:C    | 2.54                     | 0.45              |
| 3:N:1108:ARG:HE   | 3:N:1198:TYR:C    | 2.20                     | 0.45              |
| 3:N:1107:VAL:CG2  | 3:N:1219:GLU:HB3  | 2.46                     | 0.45              |
| 3:N:1223:ILE:O    | 3:N:1226:ALA:HB3  | 2.17                     | 0.45              |
| 3:N:1345:GLU:CA   | 3:N:1348:LEU:HD12 | 2.35                     | 0.45              |
| 3:N:261:LEU:HD11  | 3:N:290:PRO:O     | 2.17                     | 0.45              |
| 3:N:50:PHE:CD2    | 3:N:522:PRO:HD3   | 2.52                     | 0.45              |
| 3:N:586:ARG:O     | 3:N:587:ARG:HG2   | 2.17                     | 0.45              |
| 3:N:623:VAL:HG12  | 3:N:625:TYR:N     | 2.32                     | 0.45              |
| 3:N:85:VAL:HG21   | 3:N:89:ARG:NH2    | 2.31                     | 0.45              |
| 3:N:970:LYS:O     | 3:N:971:LEU:C     | 2.53                     | 0.45              |
| 5:P:285:GLU:HA    | 5:P:286:PRO:HD2   | 1.79                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:150:TYR:OH    | 1:B:168:ASP:HB3   | 2.16                     | 0.45              |
| 1:B:59:GLU:HB2    | 1:B:139:ASN:ND2   | 2.32                     | 0.45              |
| 2:C:176:VAL:HG11  | 2:C:182:VAL:HA    | 1.99                     | 0.45              |
| 2:C:557:ARG:O     | 2:C:560:MET:HB2   | 2.17                     | 0.45              |
| 2:C:674:VAL:HG11  | 2:C:992:MET:HB3   | 1.99                     | 0.45              |
| 2:C:953:VAL:HG13  | 2:C:966:LEU:HD13  | 1.99                     | 0.45              |
| 3:D:1149:LEU:CD2  | 3:D:1160:LEU:O    | 2.65                     | 0.45              |
| 3:D:1151:ARG:C    | 3:D:1162:GLU:CB   | 2.80                     | 0.45              |
| 3:D:119:SER:H     | 3:D:123:LEU:CB    | 2.29                     | 0.45              |
| 3:D:1254:GLN:HG2  | 3:D:1255:GLY:N    | 2.31                     | 0.45              |
| 3:D:154:THR:HG23  | 3:D:157:GLU:H     | 1.82                     | 0.45              |
| 3:D:160:GLU:O     | 3:D:161:LEU:HD23  | 2.17                     | 0.45              |
| 3:D:441:ARG:O     | 3:D:442:ASN:C     | 2.52                     | 0.45              |
| 3:D:568:ARG:O     | 3:D:569:ASN:C     | 2.55                     | 0.45              |
| 3:D:636:GLN:HA    | 3:D:636:GLN:OE1   | 2.16                     | 0.45              |
| 3:D:671:LYS:HE2   | 3:D:675:ARG:CD    | 2.47                     | 0.45              |
| 3:D:880:ILE:O     | 3:D:881:LEU:C     | 2.55                     | 0.45              |
| 4:E:19:LEU:O      | 4:E:20:THR:C      | 2.55                     | 0.45              |
| 1:K:203:GLY:C     | 1:K:205:VAL:H     | 2.20                     | 0.45              |
| 1:K:206:THR:HG23  | 1:K:207:PRO:HD2   | 1.99                     | 0.45              |
| 1:K:23:PHE:N      | 1:K:23:PHE:CD1    | 2.85                     | 0.45              |
| 1:K:73:GLU:HG2    | 1:K:130:ALA:HA    | 1.98                     | 0.45              |
| 1:L:19:GLU:HG2    | 1:L:203:GLY:CA    | 2.47                     | 0.45              |
| 2:M:148:PHE:N     | 2:M:148:PHE:CD1   | 2.84                     | 0.45              |
| 2:M:759:THR:HA    | 2:M:786:LYS:O     | 2.17                     | 0.45              |
| 1:K:63:HIS:CD2    | 2:M:801:VAL:HA    | 2.52                     | 0.45              |
| 2:M:91:GLN:HB3    | 2:M:119:PRO:HA    | 1.99                     | 0.45              |
| 3:N:1153:VAL:HG12 | 3:N:1155:VAL:HG23 | 1.99                     | 0.45              |
| 3:N:1267:ARG:NE   | 3:N:1271:LYS:NZ   | 2.63                     | 0.45              |
| 3:N:1405:GLU:OE2  | 3:N:1407:LEU:HG   | 2.16                     | 0.45              |
| 3:N:1487:VAL:O    | 4:O:73:LEU:HD12   | 2.17                     | 0.45              |
| 3:N:351:MET:HG3   | 3:N:370:ALA:HB2   | 1.98                     | 0.45              |
| 3:N:411:THR:O     | 3:N:411:THR:HG23  | 2.17                     | 0.45              |
| 3:N:554:LEU:HG    | 3:N:558:LEU:HD11  | 1.99                     | 0.45              |
| 3:N:614:PHE:CD2   | 3:N:617:ASN:ND2   | 2.85                     | 0.45              |
| 1:L:185:ARG:NH2   | 3:N:692:GLU:HG3   | 2.32                     | 0.45              |
| 3:N:796:ARG:HD2   | 3:N:862:ASP:OD2   | 2.16                     | 0.45              |
| 4:O:71:GLY:C      | 4:O:73:LEU:N      | 2.68                     | 0.45              |
| 5:P:104:ARG:HB2   | 5:P:108:GLU:OE2   | 2.16                     | 0.45              |
| 5:P:241:TRP:O     | 5:P:244:ARG:HB2   | 2.16                     | 0.45              |
| 5:P:282:LEU:O     | 5:P:284:ARG:HG2   | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:P:370:LYS:O    | 5:P:374:GLY:N    | 2.49                     | 0.45              |
| 1:A:102:LYS:HA   | 1:A:138:LEU:O    | 2.17                     | 0.45              |
| 1:A:43:ILE:HG23  | 1:A:47:SER:HB2   | 1.99                     | 0.45              |
| 1:B:13:VAL:HG23  | 1:B:22:GLU:O     | 2.17                     | 0.45              |
| 2:C:63:GLY:H     | 2:C:103:LYS:HA   | 1.81                     | 0.45              |
| 2:C:274:ARG:CZ   | 2:C:285:LEU:HD23 | 2.47                     | 0.45              |
| 2:C:477:GLY:O    | 2:C:508:ILE:HG13 | 2.16                     | 0.45              |
| 2:C:497:ALA:O    | 2:C:532:MET:HG3  | 2.16                     | 0.45              |
| 2:C:650:ARG:O    | 2:C:653:ASP:OD2  | 2.34                     | 0.45              |
| 2:C:681:GLY:O    | 2:C:684:PHE:HB2  | 2.16                     | 0.45              |
| 3:D:1000:THR:CG2 | 3:D:1036:ARG:HD2 | 2.46                     | 0.45              |
| 3:D:113:GLY:N    | 3:D:124:GLU:OE1  | 2.50                     | 0.45              |
| 3:D:1087:ARG:NH2 | 3:D:1236:LEU:O   | 2.50                     | 0.45              |
| 3:D:1305:LEU:CD2 | 3:D:1305:LEU:N   | 2.79                     | 0.45              |
| 3:D:280:ALA:HB1  | 3:D:282:TYR:OH   | 2.16                     | 0.45              |
| 3:D:428:LYS:HG2  | 3:D:429:SER:N    | 2.31                     | 0.45              |
| 3:D:614:PHE:HA   | 3:D:617:ASN:HD22 | 1.82                     | 0.45              |
| 3:D:881:LEU:O    | 3:D:882:PHE:C    | 2.55                     | 0.45              |
| 3:D:958:GLU:OE2  | 3:D:961:LYS:CG   | 2.65                     | 0.45              |
| 5:F:288:TYR:HB3  | 5:F:301:ALA:HB1  | 1.99                     | 0.45              |
| 1:K:206:THR:HG22 | 1:K:208:LEU:HB3  | 1.99                     | 0.45              |
| 1:K:54:THR:HG21  | 1:K:143:ARG:HD3  | 1.98                     | 0.45              |
| 1:L:218:LEU:O    | 1:L:221:HIS:HB2  | 2.17                     | 0.45              |
| 1:L:18:ARG:NH1   | 1:L:88:ARG:NH2   | 2.59                     | 0.45              |
| 2:M:198:ARG:NE   | 2:M:231:PRO:HG3  | 2.32                     | 0.45              |
| 2:M:365:ASP:C    | 2:M:367:LEU:H    | 2.19                     | 0.45              |
| 2:M:136:ILE:CD1  | 2:M:392:SER:HA   | 2.42                     | 0.45              |
| 2:M:572:ILE:HD12 | 2:M:701:THR:HB   | 1.98                     | 0.45              |
| 2:M:720:GLU:HG3  | 2:M:720:GLU:H    | 1.50                     | 0.45              |
| 2:M:835:VAL:O    | 2:M:835:VAL:HG13 | 2.16                     | 0.45              |
| 3:N:102:ILE:HD12 | 3:N:579:ASP:HB3  | 1.98                     | 0.45              |
| 3:N:1465:ASN:CB  | 3:N:1473:PRO:HD3 | 2.47                     | 0.45              |
| 3:N:23:TYR:CZ    | 3:N:89:ARG:NH1   | 2.85                     | 0.45              |
| 3:N:660:LYS:HD3  | 3:N:663:GLU:CD   | 2.37                     | 0.45              |
| 3:N:828:LYS:HA   | 3:N:835:SER:OG   | 2.17                     | 0.45              |
| 3:N:797:LYS:HA   | 3:N:828:LYS:O    | 2.16                     | 0.45              |
| 3:N:834:THR:HA   | 3:N:838:ARG:HD2  | 1.98                     | 0.45              |
| 3:N:793:THR:CG2  | 3:N:906:GLN:HG2  | 2.47                     | 0.45              |
| 2:M:984:GLU:CG   | 3:N:944:THR:O    | 2.65                     | 0.45              |
| 4:O:24:ALA:O     | 4:O:27:ALA:N     | 2.50                     | 0.45              |
| 5:P:163:LEU:O    | 5:P:166:LEU:HB2  | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:350:LEU:C     | 5:P:352:GLU:H     | 2.19                     | 0.45              |
| 5:P:405:LEU:HB2   | 5:P:406:ARG:H     | 1.64                     | 0.45              |
| 5:P:422:LEU:HD23  | 5:P:422:LEU:H     | 1.81                     | 0.45              |
| 1:A:9:PRO:HB2     | 1:A:25:LEU:CD1    | 2.46                     | 0.45              |
| 1:B:156:HIS:C     | 1:B:158:ILE:H     | 2.19                     | 0.45              |
| 1:B:233:VAL:C     | 1:B:235:ALA:H     | 2.20                     | 0.45              |
| 2:C:108:ILE:CG2   | 2:C:368:THR:HG21  | 2.47                     | 0.45              |
| 2:C:1092:LEU:O    | 2:C:1095:LEU:HB2  | 2.17                     | 0.45              |
| 2:C:141:HIS:CD2   | 2:C:334:ARG:CG    | 2.99                     | 0.45              |
| 2:C:327:HIS:CE1   | 2:C:329:GLY:HA3   | 2.52                     | 0.45              |
| 2:C:428:ARG:NE    | 2:C:451:LEU:HD21  | 2.31                     | 0.45              |
| 2:C:508:ILE:CD1   | 2:C:526:PRO:HB3   | 2.47                     | 0.45              |
| 2:C:842:ARG:NH2   | 2:C:887:GLU:OE2   | 2.46                     | 0.45              |
| 2:C:5:ARG:HA      | 2:C:902:ILE:HB    | 1.99                     | 0.45              |
| 3:D:1091:SER:O    | 3:D:1092:GLY:C    | 2.55                     | 0.45              |
| 3:D:1180:ALA:O    | 3:D:1181:GLY:C    | 2.55                     | 0.45              |
| 3:D:1378:TYR:CE2  | 3:D:1394:VAL:HG22 | 2.52                     | 0.45              |
| 3:D:12:LEU:HD23   | 3:D:1451:ALA:HB1  | 1.99                     | 0.45              |
| 3:D:288:MET:HG3   | 3:D:305:ALA:HB1   | 1.99                     | 0.45              |
| 3:D:480:GLU:O     | 3:D:484:PRO:HD2   | 2.17                     | 0.45              |
| 3:D:5:VAL:O       | 3:D:6:ARG:HG3     | 2.17                     | 0.45              |
| 2:C:1031:ARG:CA   | 3:D:622:ARG:NH1   | 2.80                     | 0.45              |
| 3:D:630:VAL:CG1   | 3:D:631:ILE:N     | 2.79                     | 0.45              |
| 3:D:936:TYR:HE2   | 3:D:940:THR:HG21  | 1.82                     | 0.45              |
| 5:F:204:GLY:C     | 5:F:206:GLY:N     | 2.69                     | 0.45              |
| 5:F:245:GLN:HA    | 5:F:245:GLN:NE2   | 2.26                     | 0.45              |
| 2:C:1067:TYR:HB2  | 5:F:341:PRO:CB    | 2.47                     | 0.45              |
| 1:K:44:LEU:HD21   | 1:K:214:ALA:HB2   | 1.99                     | 0.45              |
| 1:L:208:LEU:O     | 1:L:211:LEU:HB3   | 2.16                     | 0.45              |
| 1:L:89:PHE:CD2    | 1:L:94:LEU:CB     | 3.00                     | 0.45              |
| 2:M:205:GLU:N     | 2:M:209:ARG:HH11  | 2.15                     | 0.45              |
| 2:M:353:ARG:HH11  | 2:M:353:ARG:HG2   | 1.82                     | 0.45              |
| 2:M:56:GLU:HB3    | 2:M:359:MET:SD    | 2.57                     | 0.45              |
| 2:M:361:MET:N     | 2:M:361:MET:SD    | 2.73                     | 0.45              |
| 2:M:503:LEU:HD11  | 2:M:506:ASN:O     | 2.17                     | 0.45              |
| 2:M:522:VAL:CG1   | 2:M:523:ILE:N     | 2.80                     | 0.45              |
| 2:M:877:PRO:HD3   | 3:N:1023:MET:HE1  | 1.99                     | 0.45              |
| 3:N:1129:THR:HG22 | 3:N:1130:ARG:N    | 2.32                     | 0.45              |
| 3:N:1280:VAL:HG12 | 3:N:1281:VAL:N    | 2.32                     | 0.45              |
| 3:N:152:LEU:HD12  | 3:N:153:LEU:H     | 1.82                     | 0.45              |
| 2:M:1098:ASP:HB2  | 3:N:17:LYS:NZ     | 2.31                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:217:LYS:HD3   | 3:N:262:LYS:NZ    | 2.31                     | 0.45              |
| 3:N:357:GLU:N     | 3:N:357:GLU:CD    | 2.68                     | 0.45              |
| 3:N:355:VAL:HG11  | 3:N:385:VAL:HG21  | 1.99                     | 0.45              |
| 3:N:411:THR:H     | 3:N:437:VAL:HG21  | 1.82                     | 0.45              |
| 3:N:441:ARG:HG3   | 3:N:443:VAL:HG21  | 1.96                     | 0.45              |
| 3:N:596:SER:C     | 3:N:598:ARG:H     | 2.20                     | 0.45              |
| 3:N:613:ARG:O     | 3:N:614:PHE:C     | 2.55                     | 0.45              |
| 3:N:671:LYS:HE2   | 3:N:675:ARG:CG    | 2.47                     | 0.45              |
| 3:N:750:PRO:HG2   | 3:N:756:GLN:HE22  | 1.82                     | 0.45              |
| 3:N:795:VAL:CG1   | 3:N:876:SER:HB3   | 2.47                     | 0.45              |
| 5:P:250:ALA:O     | 5:P:253:ASP:HB2   | 2.17                     | 0.45              |
| 5:P:379:ARG:HH11  | 5:P:379:ARG:CG    | 2.30                     | 0.45              |
| 1:A:11:PHE:O      | 1:B:229:GLN:CB    | 2.63                     | 0.44              |
| 1:A:9:PRO:HA      | 1:A:27:PRO:HD2    | 1.99                     | 0.44              |
| 1:A:18:ARG:CD     | 1:A:88:ARG:NH2    | 2.80                     | 0.44              |
| 1:B:184:THR:HG22  | 1:B:192:LEU:O     | 2.17                     | 0.44              |
| 1:B:72:LYS:HD3    | 1:B:73:GLU:N      | 2.32                     | 0.44              |
| 2:C:18:LEU:O      | 2:C:21:ILE:CD1    | 2.65                     | 0.44              |
| 2:C:403:SER:O     | 2:C:407:LYS:HG3   | 2.18                     | 0.44              |
| 2:C:439:CYS:SG    | 2:C:442:GLU:HB2   | 2.57                     | 0.44              |
| 2:C:512:ARG:NH1   | 2:C:524:VAL:HA    | 2.28                     | 0.44              |
| 2:C:600:ASP:CB    | 2:C:650:ARG:HA    | 2.41                     | 0.44              |
| 2:C:671:ASN:C     | 2:C:672:VAL:HG12  | 2.37                     | 0.44              |
| 2:C:675:ALA:HB2   | 2:C:867:VAL:HG11  | 1.98                     | 0.44              |
| 2:C:748:GLU:HA    | 2:C:799:ILE:HG22  | 1.98                     | 0.44              |
| 2:C:953:VAL:HA    | 2:C:965:GLU:OE2   | 2.16                     | 0.44              |
| 3:D:1171:VAL:HG12 | 3:D:1175:ILE:CD1  | 2.43                     | 0.44              |
| 3:D:1173:LEU:HG   | 3:D:1174:LEU:N    | 2.31                     | 0.44              |
| 3:D:1381:VAL:CG1  | 3:D:1389:LEU:O    | 2.65                     | 0.44              |
| 3:D:175:VAL:CG1   | 3:D:193:PRO:HD2   | 2.46                     | 0.44              |
| 3:D:214:GLU:HG2   | 3:D:342:PRO:HA    | 2.00                     | 0.44              |
| 3:D:598:ARG:NH1   | 3:D:598:ARG:HG2   | 2.33                     | 0.44              |
| 5:F:355:GLU:CB    | 5:F:358:LEU:HD23  | 2.47                     | 0.44              |
| 5:F:77:THR:O      | 5:F:79:ASP:N      | 2.48                     | 0.44              |
| 5:F:85:LEU:HA     | 5:F:85:LEU:HD23   | 1.73                     | 0.44              |
| 2:M:1101:THR:O    | 2:M:1102:LEU:HD23 | 2.17                     | 0.44              |
| 2:M:235:LEU:O     | 2:M:238:LEU:HB2   | 2.17                     | 0.44              |
| 2:M:424:GLY:O     | 2:M:425:PHE:C     | 2.55                     | 0.44              |
| 2:M:504:GLU:CG    | 2:M:507:ARG:HB2   | 2.45                     | 0.44              |
| 2:M:710:ILE:HG22  | 2:M:823:VAL:HB    | 1.98                     | 0.44              |
| 2:M:709:GLU:HA    | 2:M:823:VAL:O     | 2.17                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:946:ARG:O     | 2:M:949:LYS:HB2   | 2.16                     | 0.44              |
| 3:N:1134:LEU:HD12 | 3:N:1135:ARG:H    | 1.83                     | 0.44              |
| 3:N:1205:TYR:CD2  | 3:N:1215:VAL:HG11 | 2.50                     | 0.44              |
| 3:N:1258:ARG:HH21 | 3:N:1351:GLU:CG   | 2.30                     | 0.44              |
| 3:N:223:LEU:HG    | 3:N:224:ARG:H     | 1.82                     | 0.44              |
| 3:N:130:SER:CA    | 3:N:568:ARG:NH2   | 2.80                     | 0.44              |
| 3:N:881:LEU:HG    | 3:N:885:ILE:HD11  | 2.00                     | 0.44              |
| 3:N:970:LYS:HE2   | 3:N:974:ILE:HG12  | 2.00                     | 0.44              |
| 3:N:984:THR:N     | 3:N:987:GLU:OE2   | 2.25                     | 0.44              |
| 4:O:25:LYS:O      | 4:O:28:GLN:HB2    | 2.17                     | 0.44              |
| 5:P:111:GLU:HG3   | 5:P:114:LYS:CE    | 2.47                     | 0.44              |
| 5:P:159:ILE:O     | 5:P:163:LEU:HG    | 2.17                     | 0.44              |
| 5:P:323:ASP:C     | 5:P:323:ASP:OD1   | 2.55                     | 0.44              |
| 5:P:411:HIS:CE1   | 5:P:412:GLU:OE2   | 2.70                     | 0.44              |
| 1:A:31:GLY:O      | 1:A:33:GLY:N      | 2.50                     | 0.44              |
| 1:B:104:GLU:HA    | 1:B:137:ARG:HA    | 1.98                     | 0.44              |
| 2:C:98:LEU:HD11   | 2:C:113:VAL:HG21  | 1.99                     | 0.44              |
| 2:C:95:TYR:CE2    | 2:C:114:PHE:HB3   | 2.53                     | 0.44              |
| 2:C:164:PRO:HG3   | 2:C:170:PRO:HD2   | 1.98                     | 0.44              |
| 2:C:176:VAL:HG12  | 2:C:182:VAL:CA    | 2.48                     | 0.44              |
| 2:C:293:PHE:HD1   | 2:C:294:GLU:CG    | 2.30                     | 0.44              |
| 2:C:397:GLU:OE2   | 2:C:632:ASN:N     | 2.50                     | 0.44              |
| 2:C:405:ARG:HG3   | 2:C:543:ASN:OD1   | 2.17                     | 0.44              |
| 2:C:45:GLN:O      | 2:C:48:PHE:HB2    | 2.17                     | 0.44              |
| 2:C:61:LYS:O      | 2:C:103:LYS:HB2   | 2.17                     | 0.44              |
| 2:C:63:GLY:H      | 2:C:103:LYS:CA    | 2.28                     | 0.44              |
| 2:C:861:LEU:HB2   | 2:C:863:ASP:OD1   | 2.17                     | 0.44              |
| 2:C:914:ILE:CD1   | 2:C:914:ILE:H     | 2.30                     | 0.44              |
| 3:D:1171:VAL:O    | 3:D:1175:ILE:HG13 | 2.17                     | 0.44              |
| 3:D:1324:PRO:C    | 3:D:1325:LEU:HD23 | 2.37                     | 0.44              |
| 3:D:1376:MET:HE2  | 3:D:1421:LEU:HA   | 1.98                     | 0.44              |
| 3:D:1390:LEU:O    | 3:D:1390:LEU:HD12 | 2.17                     | 0.44              |
| 3:D:186:VAL:CG1   | 3:D:187:LYS:H     | 2.29                     | 0.44              |
| 3:D:168:THR:CB    | 3:D:206:ARG:NH1   | 2.80                     | 0.44              |
| 3:D:29:PRO:O      | 3:D:30:GLU:C      | 2.55                     | 0.44              |
| 3:D:318:ARG:HG2   | 3:D:319:ALA:H     | 1.78                     | 0.44              |
| 3:D:30:GLU:CG     | 3:D:40:GLU:HG2    | 2.47                     | 0.44              |
| 3:D:591:VAL:HG21  | 3:D:597:ASP:HA    | 1.99                     | 0.44              |
| 3:D:821:VAL:HG22  | 3:D:840:LYS:HZ2   | 1.81                     | 0.44              |
| 5:F:101:GLU:HG2   | 5:F:105:LYS:HE3   | 2.00                     | 0.44              |
| 5:F:102:LEU:HD23  | 5:F:187:LEU:HB2   | 1.98                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:203:THR:CG2   | 5:F:204:GLY:N     | 2.80                     | 0.44              |
| 1:L:54:THR:HB     | 1:L:143:ARG:HD2   | 1.99                     | 0.44              |
| 2:M:1101:THR:C    | 2:M:1102:LEU:HD23 | 2.38                     | 0.44              |
| 2:M:175:GLU:O     | 2:M:176:VAL:HG13  | 2.18                     | 0.44              |
| 2:M:276:LYS:O     | 2:M:280:LYS:HG3   | 2.17                     | 0.44              |
| 2:M:443:THR:O     | 2:M:559:LEU:HD11  | 2.18                     | 0.44              |
| 2:M:47:ALA:HA     | 2:M:50:GLU:OE2    | 2.17                     | 0.44              |
| 2:M:657:ASP:CG    | 2:M:664:GLY:H     | 2.21                     | 0.44              |
| 2:M:707:ARG:HG2   | 2:M:708:TYR:N     | 2.32                     | 0.44              |
| 3:N:1018:ASN:OD1  | 3:N:1018:ASN:C    | 2.56                     | 0.44              |
| 3:N:1127:GLU:HG3  | 3:N:1128:VAL:N    | 2.29                     | 0.44              |
| 3:N:1149:LEU:HD23 | 3:N:1161:GLU:C    | 2.37                     | 0.44              |
| 3:N:1171:VAL:CA   | 3:N:1174:LEU:HD12 | 2.32                     | 0.44              |
| 3:N:1345:GLU:O    | 3:N:1346:ARG:C    | 2.55                     | 0.44              |
| 3:N:1462:LEU:O    | 3:N:1463:LYS:C    | 2.54                     | 0.44              |
| 3:N:172:PRO:HB2   | 3:N:175:VAL:CG2   | 2.48                     | 0.44              |
| 3:N:253:ALA:N     | 3:N:301:GLY:CA    | 2.74                     | 0.44              |
| 3:N:787:LEU:HD12  | 3:N:787:LEU:HA    | 1.73                     | 0.44              |
| 3:N:841:TYR:HB3   | 3:N:843:PHE:CZ    | 2.52                     | 0.44              |
| 3:N:847:ASP:OD1   | 3:N:848:GLU:N     | 2.46                     | 0.44              |
| 5:P:361:LEU:HG    | 5:P:362:SER:N     | 2.31                     | 0.44              |
| 2:C:178:PRO:C     | 2:C:180:GLY:N     | 2.69                     | 0.44              |
| 2:C:385:PHE:CD1   | 2:C:389:SER:HB2   | 2.53                     | 0.44              |
| 2:C:38:LYS:CG     | 2:C:39:ARG:N      | 2.74                     | 0.44              |
| 2:C:499:ALA:C     | 2:C:501:THR:H     | 2.20                     | 0.44              |
| 2:C:626:ARG:HG3   | 2:C:626:ARG:NH1   | 2.26                     | 0.44              |
| 2:C:683:ASN:N     | 2:C:683:ASN:HD22  | 2.11                     | 0.44              |
| 3:D:112:ILE:HG13  | 3:D:124:GLU:OE1   | 2.17                     | 0.44              |
| 3:D:1383:ASP:HA   | 3:D:1384:PRO:HD2  | 1.82                     | 0.44              |
| 3:D:325:GLU:OE2   | 3:D:332:TYR:HB3   | 2.17                     | 0.44              |
| 3:D:680:GLN:HA    | 3:D:683:ILE:HG13  | 1.99                     | 0.44              |
| 3:D:853:VAL:HG11  | 3:D:860:LEU:CD2   | 2.47                     | 0.44              |
| 3:D:930:LEU:O     | 3:D:931:LEU:C     | 2.54                     | 0.44              |
| 1:K:25:LEU:HD21   | 1:L:224:TYR:CB    | 2.47                     | 0.44              |
| 2:M:1021:LEU:HD12 | 2:M:1022:GLY:H    | 1.82                     | 0.44              |
| 2:M:157:ARG:CG    | 2:M:314:THR:HG22  | 2.47                     | 0.44              |
| 2:M:385:PHE:O     | 2:M:389:SER:HB2   | 2.17                     | 0.44              |
| 2:M:669:GLY:N     | 2:M:993:PHE:CZ    | 2.86                     | 0.44              |
| 2:M:719:PRO:CB    | 2:M:820:ARG:NH1   | 2.79                     | 0.44              |
| 2:M:731:GLU:HA    | 2:M:734:LEU:HD12  | 2.00                     | 0.44              |
| 2:M:732:ALA:HA    | 2:M:735:ARG:HG2   | 1.99                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:867:VAL:HG23  | 2:M:868:ASP:N    | 2.31                     | 0.44              |
| 2:M:69:LEU:HD22   | 2:M:97:ARG:HD3   | 2.00                     | 0.44              |
| 3:N:1274:ILE:HG22 | 3:N:1324:PRO:HA  | 1.98                     | 0.44              |
| 3:N:1344:VAL:CG1  | 3:N:1345:GLU:N   | 2.80                     | 0.44              |
| 3:N:1404:ASN:HA   | 3:N:1409:ALA:H   | 1.82                     | 0.44              |
| 3:N:284:LEU:HD12  | 3:N:290:PRO:CB   | 2.48                     | 0.44              |
| 3:N:485:SER:O     | 3:N:489:ARG:NH1  | 2.50                     | 0.44              |
| 3:N:90:MET:HG2    | 3:N:521:PRO:HD3  | 1.98                     | 0.44              |
| 3:N:527:MET:SD    | 3:N:537:THR:CG2  | 3.05                     | 0.44              |
| 3:N:732:VAL:C     | 3:N:734:GLU:H    | 2.19                     | 0.44              |
| 3:N:819:GLY:CA    | 3:N:822:ALA:HB3  | 2.45                     | 0.44              |
| 3:N:796:ARG:HG3   | 3:N:861:GLN:O    | 2.17                     | 0.44              |
| 5:P:250:ALA:O     | 5:P:251:ILE:C    | 2.56                     | 0.44              |
| 5:P:362:SER:O     | 5:P:363:GLU:C    | 2.55                     | 0.44              |
| 5:P:382:THR:HG23  | 5:P:397:ILE:HB   | 1.99                     | 0.44              |
| 1:B:61:VAL:HG13   | 1:B:163:ASN:HB3  | 2.00                     | 0.44              |
| 2:C:1096:ALA:C    | 2:C:1097:LEU:HG  | 2.37                     | 0.44              |
| 2:C:136:ILE:HD13  | 2:C:136:ILE:HA   | 1.84                     | 0.44              |
| 2:C:162:ILE:C     | 2:C:163:ILE:HG13 | 2.38                     | 0.44              |
| 2:C:546:LEU:CD2   | 2:C:583:LEU:HB2  | 2.47                     | 0.44              |
| 2:C:807:ARG:C     | 2:C:809:GLY:H    | 2.19                     | 0.44              |
| 3:D:1072:ILE:HG13 | 3:D:1072:ILE:H   | 1.45                     | 0.44              |
| 4:E:19:LEU:HD12   | 4:E:19:LEU:C     | 2.38                     | 0.44              |
| 5:F:159:ILE:HG22  | 5:F:163:LEU:HD11 | 2.00                     | 0.44              |
| 5:F:296:GLY:C     | 5:F:299:TRP:HD1  | 2.21                     | 0.44              |
| 5:F:354:LEU:HD23  | 5:F:418:LEU:HD23 | 1.98                     | 0.44              |
| 1:K:212:ASN:O     | 1:K:213:GLN:C    | 2.55                     | 0.44              |
| 1:K:9:PRO:HB2     | 1:K:25:LEU:CD1   | 2.46                     | 0.44              |
| 2:M:240:THR:O     | 2:M:242:LEU:N    | 2.51                     | 0.44              |
| 2:M:310:LEU:HD12  | 2:M:310:LEU:O    | 2.17                     | 0.44              |
| 2:M:140:ILE:HA    | 2:M:332:ARG:O    | 2.17                     | 0.44              |
| 2:M:336:VAL:O     | 2:M:337:GLY:C    | 2.56                     | 0.44              |
| 2:M:410:ILE:HG22  | 2:M:411:SER:N    | 2.31                     | 0.44              |
| 2:M:599:GLU:HG3   | 2:M:600:ASP:H    | 1.80                     | 0.44              |
| 2:M:87:ASP:HA     | 2:M:131:GLY:CA   | 2.47                     | 0.44              |
| 2:M:930:LYS:HA    | 2:M:930:LYS:HD3  | 1.64                     | 0.44              |
| 3:N:1078:ARG:O    | 3:N:1080:GLY:N   | 2.50                     | 0.44              |
| 3:N:1286:THR:HB   | 3:N:1289:LYS:O   | 2.17                     | 0.44              |
| 3:N:1353:GLN:HB3  | 3:N:1357:ARG:CZ  | 2.47                     | 0.44              |
| 3:N:148:GLU:C     | 3:N:149:LYS:HD3  | 2.36                     | 0.44              |
| 3:N:1496:GLU:OE2  | 3:N:1499:ARG:NE  | 2.51                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:444:VAL:HG23  | 3:N:444:VAL:O    | 2.17                     | 0.44              |
| 3:N:545:ARG:CZ    | 5:P:257:THR:HA   | 2.48                     | 0.44              |
| 3:N:563:PRO:CD    | 3:N:566:ILE:HD11 | 2.42                     | 0.44              |
| 3:N:563:PRO:C     | 3:N:567:ILE:HG12 | 2.38                     | 0.44              |
| 3:N:664:LYS:HB2   | 3:N:666:ILE:CD1  | 2.47                     | 0.44              |
| 1:L:185:ARG:HH22  | 3:N:692:GLU:CG   | 2.30                     | 0.44              |
| 3:N:827:ILE:HG23  | 3:N:837:GLY:CA   | 2.47                     | 0.44              |
| 3:N:885:ILE:H     | 3:N:885:ILE:HG13 | 1.65                     | 0.44              |
| 5:P:305:GLU:CG    | 5:P:309:LYS:HE3  | 2.38                     | 0.44              |
| 5:P:346:THR:O     | 5:P:349:LEU:N    | 2.50                     | 0.44              |
| 5:P:382:THR:HG22  | 5:P:394:ARG:HB2  | 1.98                     | 0.44              |
| 5:P:397:ILE:HA    | 5:P:400:ILE:HD12 | 1.98                     | 0.44              |
| 1:B:101:LEU:HB3   | 1:B:140:MET:CE   | 2.46                     | 0.44              |
| 1:B:98:THR:HA     | 1:B:142:VAL:O    | 2.17                     | 0.44              |
| 1:B:215:VAL:CG2   | 1:B:216:GLU:H    | 2.30                     | 0.44              |
| 1:B:218:LEU:O     | 1:B:221:HIS:N    | 2.50                     | 0.44              |
| 2:C:227:PHE:CA    | 2:C:237:ARG:HH12 | 2.22                     | 0.44              |
| 2:C:674:VAL:CB    | 2:C:869:VAL:HG13 | 2.48                     | 0.44              |
| 2:C:843:HIS:C     | 2:C:845:ASN:H    | 2.21                     | 0.44              |
| 3:D:1115:THR:O    | 3:D:1151:ARG:NH2 | 2.50                     | 0.44              |
| 3:D:1372:VAL:HG13 | 3:D:1375:MET:HE3 | 1.98                     | 0.44              |
| 3:D:1387:SER:HB3  | 3:D:1391:GLU:OE2 | 2.18                     | 0.44              |
| 3:D:186:VAL:HA    | 3:D:200:ASP:OD2  | 2.17                     | 0.44              |
| 3:D:223:LEU:N     | 3:D:333:LEU:O    | 2.47                     | 0.44              |
| 3:D:368:VAL:HB    | 3:D:377:VAL:CB   | 2.48                     | 0.44              |
| 3:D:417:PRO:HG2   | 3:D:428:LYS:CE   | 2.48                     | 0.44              |
| 3:D:431:VAL:HG12  | 3:D:432:TYR:N    | 2.33                     | 0.44              |
| 3:D:520:LEU:HG    | 3:D:524:LEU:HB2  | 1.99                     | 0.44              |
| 3:D:564:GLU:CD    | 3:D:564:GLU:C    | 2.76                     | 0.44              |
| 4:E:49:GLN:HG3    | 4:E:54:LEU:CD2   | 2.47                     | 0.44              |
| 5:F:222:ARG:O     | 5:F:225:GLU:HB3  | 2.17                     | 0.44              |
| 5:F:401:GLU:HG2   | 5:F:405:LEU:HD11 | 1.97                     | 0.44              |
| 2:M:102:HIS:NE2   | 2:M:108:ILE:CD1  | 2.80                     | 0.44              |
| 2:M:369:PRO:HB2   | 2:M:371:LYS:HG2  | 2.00                     | 0.44              |
| 2:M:532:MET:HG2   | 2:M:533:ASP:N    | 2.33                     | 0.44              |
| 2:M:457:ALA:N     | 2:M:540:PHE:O    | 2.50                     | 0.44              |
| 2:M:628:PHE:HA    | 2:M:638:ASP:HB3  | 1.99                     | 0.44              |
| 2:M:396:ASP:HA    | 2:M:633:GLN:NE2  | 2.32                     | 0.44              |
| 2:M:79:PRO:HG2    | 2:M:82:GLU:CB    | 2.47                     | 0.44              |
| 3:N:1048:PRO:C    | 3:N:1050:GLY:N   | 2.70                     | 0.44              |
| 3:N:1310:ARG:HD3  | 3:N:1327:ARG:HD3 | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:28:LYS:HG2    | 3:N:42:ASP:HB3    | 1.98                     | 0.44              |
| 3:N:292:VAL:HG23  | 3:N:293:VAL:N     | 2.23                     | 0.44              |
| 3:N:211:VAL:HG22  | 3:N:387:LEU:HG    | 2.00                     | 0.44              |
| 3:N:416:ALA:HB3   | 3:N:432:TYR:CD2   | 2.51                     | 0.44              |
| 3:N:408:GLU:CB    | 3:N:421:LEU:O     | 2.64                     | 0.44              |
| 3:N:502:PHE:O     | 3:N:506:GLY:N     | 2.51                     | 0.44              |
| 3:N:658:LEU:HD23  | 3:N:661:MET:CE    | 2.46                     | 0.44              |
| 3:N:792:ILE:HD12  | 3:N:881:LEU:HD23  | 1.99                     | 0.44              |
| 3:N:804:LEU:O     | 3:N:805:GLU:HG2   | 2.17                     | 0.44              |
| 3:N:819:GLY:O     | 3:N:824:ASN:ND2   | 2.51                     | 0.44              |
| 3:N:878:GLY:O     | 3:N:879:ARG:C     | 2.56                     | 0.44              |
| 4:O:81:PRO:O      | 4:O:85:LEU:CD2    | 2.66                     | 0.44              |
| 1:A:14:ARG:NH1    | 1:A:14:ARG:HG2    | 2.33                     | 0.44              |
| 1:A:205:VAL:HG12  | 1:A:206:THR:N     | 2.32                     | 0.44              |
| 1:A:24:VAL:CG1    | 1:A:25:LEU:N      | 2.80                     | 0.44              |
| 1:B:106:PRO:HA    | 1:B:133:GLU:CA    | 2.38                     | 0.44              |
| 1:B:179:PHE:HB2   | 1:B:196:THR:O     | 2.18                     | 0.44              |
| 2:C:1039:ALA:O    | 2:C:1042:ALA:HB3  | 2.17                     | 0.44              |
| 2:C:191:PHE:HD2   | 2:C:195:LEU:CD1   | 2.29                     | 0.44              |
| 2:C:322:VAL:HG12  | 2:C:323:ASP:N     | 2.31                     | 0.44              |
| 2:C:807:ARG:NH1   | 2:C:807:ARG:HB2   | 2.33                     | 0.44              |
| 3:D:1082:ALA:O    | 3:D:1083:ASP:C    | 2.56                     | 0.44              |
| 3:D:1084:THR:O    | 3:D:1085:ALA:C    | 2.56                     | 0.44              |
| 3:D:108:VAL:HA    | 3:D:110:SER:N     | 2.32                     | 0.44              |
| 3:D:1149:LEU:HD21 | 3:D:1153:VAL:HG23 | 1.99                     | 0.44              |
| 3:D:1258:ARG:NH2  | 3:D:1351:GLU:CG   | 2.81                     | 0.44              |
| 3:D:1424:VAL:O    | 3:D:1425:THR:C    | 2.55                     | 0.44              |
| 3:D:465:LEU:HD13  | 3:D:509:PRO:O     | 2.18                     | 0.44              |
| 3:D:55:ASP:HA     | 3:D:83:SER:H      | 1.83                     | 0.44              |
| 3:D:732:VAL:C     | 3:D:734:GLU:N     | 2.70                     | 0.44              |
| 3:D:832:ARG:C     | 3:D:834:THR:H     | 2.19                     | 0.44              |
| 3:D:937:TYR:O     | 3:D:938:GLY:C     | 2.56                     | 0.44              |
| 3:D:984:THR:HG22  | 3:D:987:GLU:CD    | 2.38                     | 0.44              |
| 5:F:117:SER:N     | 5:F:127:ILE:CD1   | 2.81                     | 0.44              |
| 5:F:307:THR:O     | 5:F:311:ALA:N     | 2.48                     | 0.44              |
| 1:K:183:ASP:HA    | 1:K:192:LEU:O     | 2.18                     | 0.44              |
| 1:K:23:PHE:CD2    | 1:K:211:LEU:HD23  | 2.53                     | 0.44              |
| 1:K:29:GLU:O      | 1:K:32:PHE:HB2    | 2.17                     | 0.44              |
| 1:K:65:PHE:N      | 1:K:65:PHE:CD1    | 2.85                     | 0.44              |
| 1:L:96:THR:HB     | 1:L:145:ASP:OD1   | 2.18                     | 0.44              |
| 1:L:167:VAL:CG1   | 1:L:168:ASP:N     | 2.80                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:5:LYS:NZ      | 1:L:189:ARG:NE    | 2.66                     | 0.44              |
| 1:L:241:GLU:N     | 1:L:242:PRO:CD    | 2.73                     | 0.44              |
| 2:M:1008:ARG:HD2  | 2:M:1028:GLY:C    | 2.38                     | 0.44              |
| 2:M:267:TYR:HB3   | 2:M:270:GLY:CA    | 2.47                     | 0.44              |
| 2:M:283:ILE:CG2   | 2:M:284:ARG:N     | 2.59                     | 0.44              |
| 2:M:540:PHE:HB3   | 2:M:544:THR:HG21  | 2.00                     | 0.44              |
| 3:N:1405:GLU:O    | 3:N:1410:GLU:CA   | 2.65                     | 0.44              |
| 3:N:1492:LEU:HA   | 3:N:1492:LEU:HD23 | 1.86                     | 0.44              |
| 3:N:161:LEU:N     | 3:N:161:LEU:HD23  | 2.31                     | 0.44              |
| 3:N:227:LEU:HD12  | 3:N:331:VAL:HG23  | 2.00                     | 0.44              |
| 3:N:900:ILE:HG22  | 3:N:901:GLN:N     | 2.32                     | 0.44              |
| 5:P:229:TYR:O     | 5:P:231:ARG:N     | 2.51                     | 0.44              |
| 5:P:238:TYR:CG    | 5:P:239:ALA:N     | 2.82                     | 0.44              |
| 5:P:300:ASP:HB3   | 5:P:302:LYS:CE    | 2.48                     | 0.44              |
| 1:A:26:GLU:OE1    | 1:A:194:LYS:HE3   | 2.17                     | 0.44              |
| 2:C:1068:GLU:O    | 2:C:1071:ILE:HB   | 2.17                     | 0.44              |
| 2:C:148:PHE:N     | 2:C:148:PHE:CD1   | 2.86                     | 0.44              |
| 2:C:154:ARG:C     | 2:C:156:GLY:H     | 2.21                     | 0.44              |
| 2:C:233:GLU:OE1   | 2:C:237:ARG:NH1   | 2.50                     | 0.44              |
| 2:C:139:GLN:C     | 2:C:333:ILE:HD12  | 2.38                     | 0.44              |
| 2:C:347:GLY:HA3   | 2:C:381:ALA:HB2   | 2.00                     | 0.44              |
| 2:C:115:LEU:CB    | 2:C:375:SER:HB3   | 2.42                     | 0.44              |
| 2:C:610:ARG:NH1   | 2:C:610:ARG:HG3   | 2.32                     | 0.44              |
| 2:C:720:GLU:HB3   | 2:C:760:SER:CB    | 2.41                     | 0.44              |
| 2:C:774:LEU:HA    | 2:C:777:ILE:CD1   | 2.44                     | 0.44              |
| 2:C:874:LEU:O     | 2:C:877:PRO:HD2   | 2.17                     | 0.44              |
| 2:C:984:GLU:O     | 3:D:946:GLY:HA3   | 2.18                     | 0.44              |
| 3:D:1068:LEU:O    | 3:D:1069:GLU:C    | 2.56                     | 0.44              |
| 3:D:1155:VAL:O    | 3:D:1156:LEU:C    | 2.55                     | 0.44              |
| 3:D:1160:LEU:HD22 | 3:D:1164:ARG:CD   | 2.47                     | 0.44              |
| 3:D:1253:THR:HG21 | 3:D:1258:ARG:N    | 2.32                     | 0.44              |
| 3:D:1397:LYS:CB   | 3:D:1398:TRP:HZ3  | 2.31                     | 0.44              |
| 3:D:139:GLY:O     | 3:D:147:VAL:CB    | 2.53                     | 0.44              |
| 3:D:563:PRO:C     | 3:D:565:ILE:N     | 2.71                     | 0.44              |
| 3:D:660:LYS:CG    | 3:D:694:VAL:HG22  | 2.27                     | 0.44              |
| 3:D:881:LEU:O     | 3:D:884:ARG:HB3   | 2.18                     | 0.44              |
| 3:D:884:ARG:HG3   | 3:D:888:GLU:OE2   | 2.18                     | 0.44              |
| 3:D:890:VAL:HG23  | 3:D:892:ASP:H     | 1.83                     | 0.44              |
| 3:D:910:SER:HG    | 3:D:911:LEU:H     | 1.65                     | 0.44              |
| 3:D:934:LEU:HG    | 3:D:934:LEU:H     | 1.55                     | 0.44              |
| 4:E:39:VAL:HG12   | 4:E:72:ARG:HB3    | 1.98                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:185:GLN:O    | 5:F:188:ILE:HB   | 2.17                     | 0.44              |
| 5:F:213:ILE:HG13 | 5:F:213:ILE:H    | 1.59                     | 0.44              |
| 2:M:1019:GLN:O   | 2:M:1020:PRO:C   | 2.55                     | 0.44              |
| 2:M:194:VAL:HG13 | 2:M:197:LEU:HD12 | 1.99                     | 0.44              |
| 2:M:208:ALA:HB1  | 2:M:218:VAL:HG21 | 1.99                     | 0.44              |
| 2:M:239:PHE:HE2  | 2:M:250:ARG:HD2  | 1.82                     | 0.44              |
| 2:M:136:ILE:HG22 | 2:M:336:VAL:HG22 | 1.99                     | 0.44              |
| 2:M:462:ASP:C    | 2:M:464:LEU:H    | 2.21                     | 0.44              |
| 2:M:473:ARG:NE   | 2:M:482:GLU:OE1  | 2.41                     | 0.44              |
| 2:M:52:PHE:HB3   | 2:M:53:PRO:HA    | 1.99                     | 0.44              |
| 2:M:564:MET:O    | 2:M:567:GLN:N    | 2.51                     | 0.44              |
| 2:M:640:ARG:O    | 2:M:657:ASP:N    | 2.49                     | 0.44              |
| 2:M:807:ARG:HB3  | 2:M:807:ARG:CZ   | 2.47                     | 0.44              |
| 3:N:1172:HIS:O   | 3:N:1173:LEU:C   | 2.55                     | 0.44              |
| 3:N:1191:PRO:C   | 3:N:1193:THR:N   | 2.70                     | 0.44              |
| 3:N:1405:GLU:CD  | 3:N:1406:ARG:HG3 | 2.37                     | 0.44              |
| 3:N:207:PHE:CD1  | 3:N:391:ALA:HB3  | 2.53                     | 0.44              |
| 3:N:266:GLU:OE1  | 3:N:314:PRO:HA   | 2.17                     | 0.44              |
| 3:N:400:VAL:HG22 | 3:N:402:PRO:CD   | 2.46                     | 0.44              |
| 3:N:443:VAL:HG12 | 3:N:444:VAL:N    | 2.32                     | 0.44              |
| 3:N:553:ARG:HD3  | 5:P:215:GLU:OE1  | 2.18                     | 0.44              |
| 3:N:778:LEU:HD13 | 3:N:778:LEU:HA   | 1.82                     | 0.44              |
| 3:N:960:LYS:O    | 3:N:961:LYS:C    | 2.56                     | 0.44              |
| 3:N:984:THR:HG23 | 3:N:987:GLU:H    | 1.83                     | 0.44              |
| 5:P:118:GLU:HG2  | 5:P:119:ILE:N    | 2.30                     | 0.44              |
| 5:P:373:LYS:HZ1  | 5:P:373:LYS:HB3  | 1.77                     | 0.44              |
| 1:A:69:PRO:HA    | 2:C:607:ASP:CG   | 2.39                     | 0.44              |
| 2:C:302:VAL:C    | 2:C:304:LEU:N    | 2.71                     | 0.44              |
| 2:C:280:LYS:O    | 2:C:309:TYR:CZ   | 2.71                     | 0.44              |
| 2:C:554:ASP:OD2  | 2:C:556:ASN:HB2  | 2.17                     | 0.44              |
| 2:C:575:GLN:HE21 | 2:C:670:GLN:HG2  | 1.81                     | 0.44              |
| 2:C:757:GLY:HA2  | 2:C:789:SER:CB   | 2.48                     | 0.44              |
| 2:C:580:MET:O    | 2:C:902:ILE:HA   | 2.17                     | 0.44              |
| 2:C:906:PHE:HZ   | 3:D:1070:TYR:CG  | 2.36                     | 0.44              |
| 3:D:1122:LEU:C   | 3:D:1135:ARG:HG3 | 2.37                     | 0.44              |
| 3:D:127:LEU:HD23 | 3:D:128:TYR:HA   | 2.00                     | 0.44              |
| 3:D:1280:VAL:HA  | 3:D:1317:ASP:O   | 2.18                     | 0.44              |
| 3:D:258:VAL:O    | 3:D:271:VAL:O    | 2.35                     | 0.44              |
| 3:D:274:ARG:NE   | 3:D:279:VAL:CG1  | 2.80                     | 0.44              |
| 3:D:245:LEU:N    | 3:D:309:GLY:N    | 2.61                     | 0.44              |
| 3:D:372:ASP:C    | 3:D:374:GLU:N    | 2.69                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:125:GLN:NE2  | 3:D:587:ARG:HE    | 2.12                     | 0.44              |
| 3:D:811:GLU:CB   | 3:D:815:ALA:HB3   | 2.47                     | 0.44              |
| 3:D:871:LYS:NZ   | 3:D:897:TRP:CH2   | 2.85                     | 0.44              |
| 3:D:697:GLY:HA3  | 4:E:59:ASN:ND2    | 2.33                     | 0.44              |
| 4:E:6:ILE:O      | 4:E:10:PHE:CD1    | 2.70                     | 0.44              |
| 5:F:302:LYS:HD2  | 5:F:302:LYS:C     | 2.38                     | 0.44              |
| 5:F:354:LEU:HD23 | 5:F:418:LEU:CD2   | 2.48                     | 0.44              |
| 5:F:361:LEU:CG   | 5:F:362:SER:H     | 2.31                     | 0.44              |
| 5:F:82:ARG:HA    | 5:F:85:LEU:HB2    | 1.99                     | 0.44              |
| 1:K:11:PHE:HD2   | 1:L:227:ASN:C     | 2.20                     | 0.44              |
| 1:K:57:TYR:CE1   | 1:K:163:ASN:HB2   | 2.52                     | 0.44              |
| 2:M:1101:THR:HA  | 3:N:5:VAL:HG11    | 1.99                     | 0.44              |
| 2:M:206:THR:HA   | 2:M:210:GLU:OE2   | 2.18                     | 0.44              |
| 2:M:193:LEU:HD11 | 2:M:303:PHE:HD2   | 1.82                     | 0.44              |
| 2:M:333:ILE:O    | 2:M:333:ILE:HG23  | 2.18                     | 0.44              |
| 2:M:727:PRO:HD2  | 2:M:787:ASP:HB2   | 1.99                     | 0.44              |
| 2:M:833:LEU:HA   | 2:M:833:LEU:HD12  | 1.79                     | 0.44              |
| 2:M:872:ASN:HA   | 2:M:873:PRO:HD3   | 1.80                     | 0.44              |
| 3:N:1033:GLN:NE2 | 3:N:1033:GLN:H    | 2.13                     | 0.44              |
| 3:N:362:GLU:O    | 3:N:365:ASP:HB2   | 2.17                     | 0.44              |
| 3:N:521:PRO:HB2  | 3:N:524:LEU:HG    | 2.00                     | 0.44              |
| 1:L:185:ARG:HH22 | 3:N:692:GLU:HG3   | 1.83                     | 0.44              |
| 3:N:799:LYS:HB2  | 3:N:826:PRO:CG    | 2.47                     | 0.44              |
| 5:P:233:PHE:HD1  | 5:P:233:PHE:O     | 2.01                     | 0.44              |
| 1:A:139:ASN:O    | 1:A:140:MET:HB3   | 2.17                     | 0.44              |
| 1:A:1:MET:CA     | 1:A:6:LEU:HD22    | 2.48                     | 0.44              |
| 1:B:55:SER:HB3   | 1:B:166:PRO:HA    | 2.00                     | 0.44              |
| 2:C:1104:GLU:C   | 2:C:1106:ASP:N    | 2.71                     | 0.44              |
| 2:C:260:LEU:CB   | 2:C:291:ALA:HB2   | 2.47                     | 0.44              |
| 2:C:336:VAL:N    | 2:C:339:LEU:HD12  | 2.32                     | 0.44              |
| 2:C:589:ARG:O    | 2:C:592:LEU:HD23  | 2.18                     | 0.44              |
| 2:C:60:GLY:C     | 2:C:62:GLY:N      | 2.68                     | 0.44              |
| 2:C:626:ARG:CG   | 2:C:626:ARG:NH1   | 2.81                     | 0.44              |
| 2:C:832:LYS:HG2  | 2:C:833:LEU:N     | 2.33                     | 0.44              |
| 2:C:853:LEU:HA   | 2:C:854:PRO:HD3   | 1.80                     | 0.44              |
| 2:C:984:GLU:CD   | 3:D:791:TYR:HE2   | 2.21                     | 0.44              |
| 3:D:1059:SER:HB2 | 3:D:1065:LEU:HD22 | 2.00                     | 0.44              |
| 3:D:100:ALA:CB   | 3:D:128:TYR:CE2   | 3.00                     | 0.44              |
| 3:D:1346:ARG:NH1 | 3:D:1346:ARG:HG3  | 2.32                     | 0.44              |
| 3:D:35:ARG:HG3   | 3:D:36:THR:OG1    | 2.18                     | 0.44              |
| 3:D:36:THR:CG2   | 3:D:38:LYS:HE2    | 2.48                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:99:ALA:HB1    | 3:D:578:VAL:HG21 | 2.00                     | 0.44              |
| 3:D:800:LYS:HZ2   | 3:D:825:ALA:HA   | 1.83                     | 0.44              |
| 3:D:871:LYS:HG2   | 3:D:873:LEU:HD21 | 1.99                     | 0.44              |
| 3:D:920:LEU:O     | 3:D:921:ARG:C    | 2.57                     | 0.44              |
| 3:D:931:LEU:O     | 3:D:934:LEU:HB2  | 2.17                     | 0.44              |
| 4:E:39:VAL:O      | 4:E:72:ARG:HD2   | 2.17                     | 0.44              |
| 3:D:1489:GLN:HE22 | 4:E:72:ARG:HA    | 1.83                     | 0.44              |
| 4:E:81:PRO:O      | 4:E:85:LEU:HD21  | 2.17                     | 0.44              |
| 5:F:102:LEU:O     | 5:F:105:LYS:HB2  | 2.18                     | 0.44              |
| 5:F:184:ARG:O     | 5:F:185:GLN:C    | 2.55                     | 0.44              |
| 5:F:256:ARG:HH11  | 5:F:256:ARG:HG2  | 1.83                     | 0.44              |
| 5:F:348:SER:OG    | 5:F:349:LEU:N    | 2.51                     | 0.44              |
| 5:F:83:GLN:O      | 5:F:84:TYR:C     | 2.55                     | 0.44              |
| 1:K:73:GLU:HB3    | 1:K:78:ILE:CG1   | 2.47                     | 0.44              |
| 1:L:185:ARG:HB3   | 1:L:190:THR:HG23 | 2.00                     | 0.44              |
| 2:M:1060:ILE:HG13 | 2:M:1083:GLU:CG  | 2.48                     | 0.44              |
| 2:M:208:ALA:HB1   | 2:M:218:VAL:CG2  | 2.47                     | 0.44              |
| 2:M:236:ILE:O     | 2:M:237:ARG:C    | 2.56                     | 0.44              |
| 2:M:334:ARG:CB    | 2:M:339:LEU:HD21 | 2.45                     | 0.44              |
| 2:M:477:GLY:O     | 2:M:507:ARG:HA   | 2.17                     | 0.44              |
| 2:M:588:VAL:CG2   | 2:M:589:ARG:H    | 2.29                     | 0.44              |
| 2:M:677:MET:HB2   | 2:M:678:PRO:HD2  | 2.00                     | 0.44              |
| 3:N:1091:SER:O    | 3:N:1093:TYR:N   | 2.50                     | 0.44              |
| 3:N:122:GLU:O     | 3:N:126:VAL:CG2  | 2.66                     | 0.44              |
| 3:N:1267:ARG:NH2  | 3:N:1271:LYS:NZ  | 2.53                     | 0.44              |
| 3:N:1321:ALA:O    | 3:N:1339:LYS:HE3 | 2.17                     | 0.44              |
| 3:N:1372:VAL:HG13 | 3:N:1375:MET:HE3 | 1.99                     | 0.44              |
| 3:N:1404:ASN:CA   | 3:N:1409:ALA:H   | 2.31                     | 0.44              |
| 3:N:1476:THR:CG2  | 4:O:17:TYR:HB3   | 2.48                     | 0.44              |
| 3:N:664:LYS:O     | 3:N:665:GLY:C    | 2.56                     | 0.44              |
| 3:N:804:LEU:HD23  | 3:N:804:LEU:HA   | 1.75                     | 0.44              |
| 3:N:806:PHE:HE1   | 3:N:816:HIS:NE2  | 2.16                     | 0.44              |
| 5:P:100:VAL:O     | 5:P:101:GLU:C    | 2.55                     | 0.44              |
| 5:P:291:ILE:O     | 5:P:291:ILE:HD12 | 2.18                     | 0.44              |
| 5:P:408:LEU:HD12  | 5:P:411:HIS:CE1  | 2.53                     | 0.44              |
| 1:A:104:GLU:HA    | 1:A:137:ARG:HA   | 2.00                     | 0.43              |
| 1:B:13:VAL:HG21   | 1:B:23:PHE:CD2   | 2.53                     | 0.43              |
| 1:B:38:ASN:HB3    | 1:B:39:PRO:CD    | 2.34                     | 0.43              |
| 2:C:1015:LEU:HD13 | 5:F:335:ASP:HA   | 1.99                     | 0.43              |
| 2:C:193:LEU:HD23  | 2:C:307:LEU:HD22 | 2.00                     | 0.43              |
| 2:C:713:ARG:NH2   | 2:C:758:ARG:HH12 | 2.15                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1029:ARG:CG   | 3:D:1029:ARG:HH11 | 2.14                     | 0.43              |
| 3:D:1038:LEU:HD23 | 3:D:1061:PHE:CB   | 2.47                     | 0.43              |
| 3:D:1274:ILE:HA   | 3:D:1325:LEU:HG   | 2.00                     | 0.43              |
| 3:D:1286:THR:C    | 3:D:1288:GLU:N    | 2.70                     | 0.43              |
| 3:D:1286:THR:HG22 | 3:D:1288:GLU:HB2  | 2.00                     | 0.43              |
| 3:D:1347:TYR:CZ   | 3:D:1351:GLU:HG2  | 2.53                     | 0.43              |
| 3:D:142:LEU:HD13  | 3:D:144:GLY:N     | 2.33                     | 0.43              |
| 3:D:284:LEU:HD22  | 3:D:288:MET:HG2   | 1.99                     | 0.43              |
| 3:D:244:GLU:CD    | 3:D:310:LEU:HD23  | 2.38                     | 0.43              |
| 3:D:566:ILE:HG13  | 3:D:567:ILE:N     | 2.33                     | 0.43              |
| 3:D:579:ASP:O     | 3:D:580:ALA:C     | 2.56                     | 0.43              |
| 3:D:921:ARG:HH11  | 3:D:921:ARG:HA    | 1.82                     | 0.43              |
| 3:D:953:ASP:C     | 3:D:955:VAL:N     | 2.72                     | 0.43              |
| 3:D:959:GLU:O     | 3:D:962:GLN:HB2   | 2.18                     | 0.43              |
| 3:D:985:ASP:N     | 3:D:985:ASP:OD2   | 2.46                     | 0.43              |
| 5:F:136:LEU:HB3   | 5:F:140:ARG:HD3   | 2.00                     | 0.43              |
| 1:K:99:LEU:CB     | 1:K:114:PHE:CD2   | 3.00                     | 0.43              |
| 1:K:127:LEU:HD12  | 1:K:128:HIS:N     | 2.33                     | 0.43              |
| 1:K:186:LEU:O     | 1:K:186:LEU:HG    | 2.18                     | 0.43              |
| 1:L:104:GLU:HA    | 1:L:132:LEU:HD13  | 2.00                     | 0.43              |
| 1:L:54:THR:OG1    | 1:L:145:ASP:HB2   | 2.17                     | 0.43              |
| 1:L:13:VAL:CG2    | 1:L:14:ARG:N      | 2.81                     | 0.43              |
| 2:M:264:PRO:HB2   | 2:M:289:THR:CB    | 2.46                     | 0.43              |
| 3:N:1091:SER:C    | 3:N:1093:TYR:H    | 2.18                     | 0.43              |
| 3:N:1126:ASP:OD1  | 3:N:1126:ASP:O    | 2.35                     | 0.43              |
| 3:N:1191:PRO:C    | 3:N:1193:THR:H    | 2.20                     | 0.43              |
| 3:N:399:ARG:HD3   | 3:N:399:ARG:HA    | 1.76                     | 0.43              |
| 3:N:400:VAL:HG23  | 3:N:443:VAL:HG11  | 1.98                     | 0.43              |
| 3:N:414:ARG:O     | 3:N:415:VAL:CG1   | 2.66                     | 0.43              |
| 3:N:485:SER:C     | 3:N:489:ARG:HD3   | 2.36                     | 0.43              |
| 3:N:492:ALA:O     | 3:N:493:ARG:C     | 2.55                     | 0.43              |
| 3:N:803:GLY:C     | 3:N:805:GLU:H     | 2.21                     | 0.43              |
| 3:N:919:PHE:CD1   | 3:N:919:PHE:C     | 2.91                     | 0.43              |
| 5:P:245:GLN:O     | 5:P:246:ALA:C     | 2.56                     | 0.43              |
| 5:P:267:THR:O     | 5:P:270:LYS:HB3   | 2.18                     | 0.43              |
| 5:P:268:ILE:HA    | 5:P:271:LEU:HG    | 1.99                     | 0.43              |
| 5:P:370:LYS:O     | 5:P:371:LEU:C     | 2.55                     | 0.43              |
| 5:P:380:GLU:HA    | 5:P:385:GLU:OE2   | 2.17                     | 0.43              |
| 1:A:161:ARG:H     | 1:A:164:ALA:HB2   | 1.83                     | 0.43              |
| 2:C:1085:PHE:CD1  | 2:C:1085:PHE:C    | 2.91                     | 0.43              |
| 2:C:157:ARG:CG    | 2:C:158:TYR:N     | 2.81                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:198:ARG:HE    | 2:C:231:PRO:CG    | 2.31                     | 0.43              |
| 2:C:273:GLY:HA2   | 2:C:276:LYS:CG    | 2.48                     | 0.43              |
| 2:C:384:GLU:OE2   | 2:C:384:GLU:HA    | 2.17                     | 0.43              |
| 2:C:470:PRO:CB    | 2:C:534:VAL:HG21  | 2.48                     | 0.43              |
| 2:C:601:GLY:O     | 2:C:648:ARG:HA    | 2.17                     | 0.43              |
| 2:C:750:LYS:O     | 2:C:751:PRO:C     | 2.55                     | 0.43              |
| 2:C:815:LEU:HD21  | 2:C:822:VAL:HG22  | 1.99                     | 0.43              |
| 2:C:826:TYR:CD1   | 2:C:826:TYR:N     | 2.87                     | 0.43              |
| 2:C:78:PHE:HD2    | 2:C:82:GLU:OE2    | 2.01                     | 0.43              |
| 2:C:833:LEU:HD12  | 2:C:833:LEU:HA    | 1.81                     | 0.43              |
| 3:D:1000:THR:HG22 | 3:D:1036:ARG:HD2  | 1.99                     | 0.43              |
| 3:D:1087:ARG:HD2  | 3:D:1234:THR:CA   | 2.48                     | 0.43              |
| 3:D:1132:LEU:HA   | 3:D:1132:LEU:HD12 | 1.74                     | 0.43              |
| 3:D:1209:LEU:HD23 | 3:D:1209:LEU:HA   | 1.81                     | 0.43              |
| 3:D:1087:ARG:HB3  | 3:D:1234:THR:HA   | 1.99                     | 0.43              |
| 3:D:1286:THR:CG2  | 3:D:1288:GLU:HB2  | 2.48                     | 0.43              |
| 3:D:1366:LYS:O    | 3:D:1367:HIS:C    | 2.56                     | 0.43              |
| 3:D:1443:THR:CG2  | 10:D:1529:NE6:H24 | 2.47                     | 0.43              |
| 3:D:1450:ALA:HA   | 3:D:1455:LYS:HG3  | 1.99                     | 0.43              |
| 3:D:1467:ILE:HD11 | 10:D:1529:NE6:C19 | 2.48                     | 0.43              |
| 3:D:241:ILE:CG1   | 3:D:312:ARG:HG2   | 2.48                     | 0.43              |
| 3:D:675:ARG:O     | 3:D:677:LEU:N     | 2.51                     | 0.43              |
| 3:D:711:LEU:C     | 3:D:713:ILE:N     | 2.71                     | 0.43              |
| 3:D:701:LEU:HD23  | 3:D:715:ALA:HB2   | 1.98                     | 0.43              |
| 3:D:787:LEU:O     | 3:D:788:GLY:C     | 2.56                     | 0.43              |
| 3:D:815:ALA:O     | 3:D:818:ARG:HB2   | 2.18                     | 0.43              |
| 4:E:73:LEU:HD12   | 4:E:74:VAL:N      | 2.31                     | 0.43              |
| 5:F:401:GLU:O     | 5:F:402:ASN:C     | 2.56                     | 0.43              |
| 5:F:79:ASP:HB2    | 5:F:81:VAL:CG2    | 2.47                     | 0.43              |
| 1:K:56:VAL:HG22   | 1:K:142:VAL:HG13  | 2.00                     | 0.43              |
| 1:L:86:VAL:HG22   | 1:L:123:MET:CG    | 2.48                     | 0.43              |
| 1:L:208:LEU:CD1   | 1:L:212:ASN:HD21  | 2.31                     | 0.43              |
| 1:L:5:LYS:HA      | 1:L:5:LYS:HD3     | 1.81                     | 0.43              |
| 1:L:82:LEU:N      | 1:L:82:LEU:HD23   | 2.33                     | 0.43              |
| 2:M:1000:MET:HB3  | 2:M:1002:GLU:HG3  | 2.00                     | 0.43              |
| 2:M:409:ARG:C     | 2:M:410:ILE:HD12  | 2.38                     | 0.43              |
| 2:M:571:LEU:HD22  | 2:M:701:THR:N     | 2.33                     | 0.43              |
| 2:M:750:LYS:O     | 2:M:751:PRO:C     | 2.55                     | 0.43              |
| 2:M:854:PRO:HD2   | 2:M:857:ASP:OD1   | 2.18                     | 0.43              |
| 2:M:576:ALA:HB3   | 2:M:900:ARG:HH12  | 1.83                     | 0.43              |
| 2:M:914:ILE:O     | 2:M:917:LEU:N     | 2.51                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:928:LYS:HG2  | 2:M:928:LYS:O    | 2.19                     | 0.43              |
| 3:N:1006:ALA:O   | 3:N:1007:VAL:C   | 2.57                     | 0.43              |
| 3:N:102:ILE:O    | 3:N:105:VAL:N    | 2.51                     | 0.43              |
| 3:N:154:THR:HG23 | 3:N:156:GLU:HG2  | 2.00                     | 0.43              |
| 3:N:256:GLU:HB2  | 3:N:296:GLU:CG   | 2.47                     | 0.43              |
| 3:N:437:VAL:HB   | 5:P:179:GLU:OE2  | 2.18                     | 0.43              |
| 3:N:494:LYS:HA   | 3:N:1388:ARG:NH1 | 2.23                     | 0.43              |
| 3:N:692:GLU:O    | 3:N:695:ILE:N    | 2.51                     | 0.43              |
| 3:N:903:ASP:O    | 3:N:904:VAL:HG13 | 2.18                     | 0.43              |
| 3:N:912:LYS:HB3  | 3:N:912:LYS:NZ   | 2.21                     | 0.43              |
| 4:O:39:VAL:HG12  | 4:O:39:VAL:O     | 2.18                     | 0.43              |
| 5:P:188:ILE:O    | 5:P:189:GLU:C    | 2.56                     | 0.43              |
| 5:P:288:TYR:HB3  | 5:P:301:ALA:HA   | 2.01                     | 0.43              |
| 5:P:355:GLU:HA   | 5:P:358:LEU:CD2  | 2.48                     | 0.43              |
| 5:P:410:TYR:HA   | 5:P:413:SER:OG   | 2.19                     | 0.43              |
| 5:P:421:PHE:CD1  | 5:P:422:LEU:N    | 2.86                     | 0.43              |
| 1:B:100:LEU:HB3  | 1:B:115:LEU:HD22 | 1.99                     | 0.43              |
| 2:C:265:ARG:HA   | 2:C:289:THR:OG1  | 2.18                     | 0.43              |
| 2:C:329:GLY:HA3  | 2:C:489:THR:HG23 | 2.00                     | 0.43              |
| 2:C:368:THR:HB   | 2:C:369:PRO:CD   | 2.27                     | 0.43              |
| 2:C:41:ASN:HD22  | 2:C:42:VAL:N     | 2.16                     | 0.43              |
| 2:C:504:GLU:HG3  | 2:C:507:ARG:HD3  | 2.00                     | 0.43              |
| 2:C:55:GLU:HG2   | 2:C:56:GLU:N     | 2.33                     | 0.43              |
| 2:C:685:GLU:C    | 2:C:687:ALA:H    | 2.20                     | 0.43              |
| 2:C:693:GLU:HG3  | 2:C:697:ARG:NH1  | 2.32                     | 0.43              |
| 2:C:694:LEU:HD23 | 2:C:697:ARG:HH22 | 1.82                     | 0.43              |
| 2:C:783:ARG:C    | 2:C:785:VAL:H    | 2.21                     | 0.43              |
| 2:C:673:LEU:N    | 2:C:868:ASP:OD2  | 2.47                     | 0.43              |
| 2:C:876:VAL:O    | 2:C:879:ARG:N    | 2.46                     | 0.43              |
| 3:D:1011:PHE:CD1 | 3:D:1021:TYR:HB2 | 2.53                     | 0.43              |
| 3:D:1145:TYR:CD2 | 3:D:1146:GLY:N   | 2.87                     | 0.43              |
| 3:D:257:GLY:CA   | 3:D:274:ARG:CA   | 2.93                     | 0.43              |
| 3:D:354:VAL:CB   | 3:D:367:ILE:O    | 2.65                     | 0.43              |
| 3:D:500:ARG:O    | 3:D:504:ASP:CB   | 2.66                     | 0.43              |
| 3:D:520:LEU:HD21 | 3:D:524:LEU:HB2  | 1.98                     | 0.43              |
| 3:D:623:VAL:CG1  | 3:D:624:ASP:N    | 2.81                     | 0.43              |
| 3:D:788:GLY:O    | 3:D:791:TYR:HB3  | 2.18                     | 0.43              |
| 3:D:887:ALA:CA   | 3:D:890:VAL:HG22 | 2.48                     | 0.43              |
| 4:E:21:VAL:O     | 4:E:24:ALA:HB3   | 2.19                     | 0.43              |
| 4:E:81:PRO:O     | 4:E:85:LEU:CD2   | 2.66                     | 0.43              |
| 5:F:100:VAL:O    | 5:F:101:GLU:C    | 2.55                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:410:TYR:O     | 5:F:413:SER:HB2   | 2.18                     | 0.43              |
| 1:K:38:ASN:O      | 1:K:39:PRO:C      | 2.56                     | 0.43              |
| 1:K:1:MET:HA      | 1:K:6:LEU:HD22    | 2.00                     | 0.43              |
| 1:L:42:ARG:HH22   | 2:M:939:ARG:HH21  | 1.66                     | 0.43              |
| 2:M:175:GLU:O     | 2:M:183:SER:HB2   | 2.19                     | 0.43              |
| 2:M:192:PRO:O     | 2:M:193:LEU:C     | 2.56                     | 0.43              |
| 2:M:406:HIS:HA    | 2:M:409:ARG:HD2   | 2.00                     | 0.43              |
| 2:M:410:ILE:N     | 2:M:453:THR:O     | 2.51                     | 0.43              |
| 2:M:54:ILE:O      | 2:M:54:ILE:HG23   | 2.17                     | 0.43              |
| 2:M:599:GLU:HB3   | 2:M:615:TYR:CE2   | 2.53                     | 0.43              |
| 2:M:815:LEU:HD13  | 2:M:819:VAL:HG12  | 2.00                     | 0.43              |
| 2:M:910:LYS:O     | 2:M:911:GLU:C     | 2.57                     | 0.43              |
| 3:N:1481:VAL:HG12 | 4:O:21:VAL:HG21   | 2.01                     | 0.43              |
| 3:N:1491:THR:O    | 3:N:1491:THR:HG22 | 2.17                     | 0.43              |
| 3:N:223:LEU:C     | 3:N:332:TYR:HA    | 2.39                     | 0.43              |
| 3:N:85:VAL:CG2    | 3:N:89:ARG:CZ     | 2.91                     | 0.43              |
| 2:M:676:ILE:HD13  | 3:N:949:ILE:H     | 1.83                     | 0.43              |
| 3:N:990:ASP:HA    | 3:N:993:LEU:HG    | 2.00                     | 0.43              |
| 5:P:352:GLU:CA    | 5:P:355:GLU:OE2   | 2.57                     | 0.43              |
| 5:P:367:MET:HE2   | 5:P:371:LEU:HD21  | 1.99                     | 0.43              |
| 5:P:386:VAL:HG11  | 5:P:394:ARG:N     | 2.33                     | 0.43              |
| 1:B:188:GLN:CG    | 1:B:189:ARG:HG3   | 2.47                     | 0.43              |
| 2:C:18:LEU:O      | 2:C:21:ILE:HD13   | 2.18                     | 0.43              |
| 2:C:191:PHE:CD2   | 2:C:195:LEU:CD1   | 3.01                     | 0.43              |
| 2:C:20:GLU:CA     | 2:C:23:VAL:HG22   | 2.47                     | 0.43              |
| 2:C:517:ARG:O     | 2:C:520:GLU:CB    | 2.67                     | 0.43              |
| 2:C:583:LEU:O     | 2:C:586:ARG:N     | 2.51                     | 0.43              |
| 2:C:807:ARG:O     | 2:C:808:ARG:C     | 2.56                     | 0.43              |
| 2:C:809:GLY:HA3   | 2:C:813:VAL:CG2   | 2.48                     | 0.43              |
| 3:D:1008:PHE:H    | 3:D:1008:PHE:HD1  | 1.66                     | 0.43              |
| 3:D:1221:VAL:HG12 | 3:D:1370:ILE:HD13 | 2.01                     | 0.43              |
| 3:D:1404:ASN:OD1  | 3:D:1408:ILE:HG22 | 2.18                     | 0.43              |
| 3:D:28:LYS:HE2    | 3:D:42:ASP:HB3    | 2.00                     | 0.43              |
| 3:D:553:ARG:HG2   | 3:D:557:LEU:HD11  | 1.99                     | 0.43              |
| 3:D:106:LYS:HB3   | 3:D:586:ARG:NH1   | 2.32                     | 0.43              |
| 3:D:761:ILE:CD1   | 4:E:20:THR:HA     | 2.49                     | 0.43              |
| 3:D:810:GLU:C     | 3:D:812:ALA:H     | 2.21                     | 0.43              |
| 3:D:819:GLY:HA2   | 3:D:822:ALA:HB3   | 1.98                     | 0.43              |
| 3:D:907:GLU:OE1   | 3:D:909:ASN:N     | 2.51                     | 0.43              |
| 3:D:95:LEU:HB3    | 3:D:97:THR:O      | 2.19                     | 0.43              |
| 5:F:107:GLU:OE2   | 5:F:229:TYR:CD1   | 2.71                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:231:ARG:HB3   | 5:F:233:PHE:HE2   | 1.83                     | 0.43              |
| 1:K:124:ASN:CB    | 1:K:127:LEU:HB2   | 2.48                     | 0.43              |
| 1:L:114:PHE:O     | 1:L:116:PRO:HD3   | 2.18                     | 0.43              |
| 1:K:34:VAL:CB     | 1:L:42:ARG:NH1    | 2.79                     | 0.43              |
| 1:L:78:ILE:O      | 1:L:81:ASN:HB2    | 2.18                     | 0.43              |
| 2:M:204:GLN:CD    | 2:M:225:SER:HA    | 2.38                     | 0.43              |
| 2:M:289:THR:HG22  | 2:M:290:LEU:CD2   | 2.48                     | 0.43              |
| 2:M:559:LEU:HG    | 2:M:560:MET:N     | 2.31                     | 0.43              |
| 2:M:562:SER:O     | 2:M:563:ASN:C     | 2.56                     | 0.43              |
| 2:M:581:THR:N     | 2:M:584:GLU:OE2   | 2.51                     | 0.43              |
| 2:M:690:ILE:CG2   | 2:M:691:SER:N     | 2.81                     | 0.43              |
| 2:M:768:THR:HB    | 2:M:771:GLU:CB    | 2.48                     | 0.43              |
| 2:M:576:ALA:HB3   | 2:M:900:ARG:NH1   | 2.33                     | 0.43              |
| 3:N:1047:LYS:N    | 3:N:1051:GLU:O    | 2.46                     | 0.43              |
| 3:N:130:SER:N     | 3:N:568:ARG:HH21  | 2.15                     | 0.43              |
| 3:N:1324:PRO:C    | 3:N:1325:LEU:HD23 | 2.39                     | 0.43              |
| 3:N:1451:ALA:O    | 3:N:1454:GLY:N    | 2.51                     | 0.43              |
| 3:N:1488:ASP:C    | 3:N:1490:LYS:N    | 2.71                     | 0.43              |
| 3:N:408:GLU:OE2   | 3:N:444:VAL:HG11  | 2.18                     | 0.43              |
| 3:N:473:LEU:O     | 3:N:476:GLU:HB3   | 2.18                     | 0.43              |
| 3:N:539:ASP:H     | 5:P:318:GLU:CD    | 2.21                     | 0.43              |
| 3:N:573:MET:CE    | 5:P:210:LEU:HB2   | 2.48                     | 0.43              |
| 3:N:634:GLY:HA3   | 3:N:637:LEU:CG    | 2.47                     | 0.43              |
| 3:N:970:LYS:HA    | 3:N:973:GLN:NE2   | 2.34                     | 0.43              |
| 5:P:238:TYR:O     | 5:P:240:THR:N     | 2.51                     | 0.43              |
| 5:P:276:ARG:C     | 5:P:278:LEU:H     | 2.22                     | 0.43              |
| 5:P:289:GLU:N     | 5:P:289:GLU:CD    | 2.69                     | 0.43              |
| 5:P:328:PHE:CD1   | 5:P:328:PHE:N     | 2.87                     | 0.43              |
| 5:P:373:LYS:HE3   | 5:P:379:ARG:HB3   | 2.00                     | 0.43              |
| 2:C:105:THR:O     | 2:C:107:LEU:HG    | 2.17                     | 0.43              |
| 2:C:195:LEU:O     | 2:C:199:VAL:HG23  | 2.18                     | 0.43              |
| 2:C:227:PHE:N     | 2:C:227:PHE:CD1   | 2.86                     | 0.43              |
| 2:C:110:GLU:CB    | 2:C:369:PRO:HB3   | 2.48                     | 0.43              |
| 2:C:458:TYR:HB2   | 2:C:538:GLN:HA    | 2.00                     | 0.43              |
| 3:D:1031:ASN:HB2  | 3:D:1032:PRO:HD2  | 1.99                     | 0.43              |
| 3:D:1066:THR:HB   | 3:D:1069:GLU:CB   | 2.48                     | 0.43              |
| 3:D:1280:VAL:CG1  | 3:D:1281:VAL:N    | 2.81                     | 0.43              |
| 3:D:1495:ILE:HG13 | 4:E:84:ARG:HH11   | 1.78                     | 0.43              |
| 3:D:36:THR:HG22   | 3:D:38:LYS:HE2    | 2.01                     | 0.43              |
| 3:D:408:GLU:HG3   | 3:D:422:ALA:N     | 2.34                     | 0.43              |
| 3:D:522:PRO:O     | 3:D:524:LEU:N     | 2.51                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:59:ALA:C     | 3:D:61:GLY:H      | 2.22                     | 0.43              |
| 3:D:629:SER:HB3  | 3:D:726:ILE:CD1   | 2.49                     | 0.43              |
| 3:D:754:PHE:O    | 3:D:757:ALA:HB3   | 2.18                     | 0.43              |
| 3:D:801:GLY:HA2  | 3:D:830:ALA:HB3   | 2.01                     | 0.43              |
| 3:D:909:ASN:O    | 3:D:912:LYS:N     | 2.52                     | 0.43              |
| 4:E:5:GLY:O      | 4:E:6:ILE:C       | 2.57                     | 0.43              |
| 5:F:157:GLU:O    | 5:F:158:GLU:C     | 2.56                     | 0.43              |
| 3:D:34:TYR:HE2   | 5:F:261:PRO:HD3   | 1.83                     | 0.43              |
| 1:K:179:PHE:HB2  | 1:K:195:LEU:HD11  | 2.00                     | 0.43              |
| 1:L:211:LEU:O    | 1:L:212:ASN:C     | 2.56                     | 0.43              |
| 1:L:215:VAL:HG23 | 1:L:216:GLU:N     | 2.32                     | 0.43              |
| 2:M:1055:LEU:CG  | 2:M:1079:PRO:HG3  | 2.48                     | 0.43              |
| 2:M:1087:VAL:O   | 2:M:1090:LYS:HB2  | 2.18                     | 0.43              |
| 2:M:185:LYS:HE2  | 2:M:190:LYS:HZ2   | 1.84                     | 0.43              |
| 2:M:247:PRO:HA   | 2:M:248:PRO:HD3   | 1.75                     | 0.43              |
| 2:M:334:ARG:HH11 | 2:M:418:LEU:CD1   | 2.30                     | 0.43              |
| 2:M:691:SER:O    | 2:M:692:GLU:C     | 2.57                     | 0.43              |
| 2:M:731:GLU:C    | 2:M:733:ALA:H     | 2.21                     | 0.43              |
| 2:M:961:GLU:OE2  | 2:M:964:LYS:HB3   | 2.19                     | 0.43              |
| 2:M:971:LYS:NZ   | 3:N:950:GLY:HA3   | 2.33                     | 0.43              |
| 2:M:857:ASP:HB2  | 2:M:978:ARG:HG2   | 1.99                     | 0.43              |
| 3:N:1174:LEU:O   | 3:N:1177:ALA:HB3  | 2.19                     | 0.43              |
| 3:N:1260:ILE:O   | 3:N:1261:GLU:C    | 2.57                     | 0.43              |
| 3:N:1434:TRP:NE1 | 3:N:1435:LEU:HD23 | 2.33                     | 0.43              |
| 3:N:197:SER:OG   | 3:N:199:LEU:O     | 2.36                     | 0.43              |
| 3:N:274:ARG:C    | 3:N:275:GLU:HG3   | 2.39                     | 0.43              |
| 3:N:573:MET:O    | 3:N:574:LEU:C     | 2.56                     | 0.43              |
| 3:N:664:LYS:O    | 3:N:666:ILE:N     | 2.52                     | 0.43              |
| 5:P:127:ILE:O    | 5:P:130:VAL:N     | 2.45                     | 0.43              |
| 5:P:225:GLU:O    | 5:P:227:PHE:N     | 2.51                     | 0.43              |
| 5:P:385:GLU:O    | 5:P:388:ALA:HB3   | 2.19                     | 0.43              |
| 1:A:191:ASP:O    | 2:C:938:LYS:NZ    | 2.51                     | 0.43              |
| 1:A:5:LYS:C      | 1:A:7:LYS:N       | 2.72                     | 0.43              |
| 1:B:80:LEU:HB3   | 3:D:844:ALA:CB    | 2.49                     | 0.43              |
| 2:C:1051:GLU:OE2 | 2:C:1056:LYS:HE3  | 2.18                     | 0.43              |
| 2:C:151:ASP:H    | 2:C:158:TYR:CB    | 2.31                     | 0.43              |
| 2:C:285:LEU:HD11 | 2:C:289:THR:HA    | 2.01                     | 0.43              |
| 2:C:342:ASP:OD1  | 2:C:343:GLN:N     | 2.51                     | 0.43              |
| 2:C:353:ARG:CG   | 2:C:353:ARG:NH1   | 2.80                     | 0.43              |
| 2:C:861:LEU:HG   | 2:C:865:THR:OG1   | 2.18                     | 0.43              |
| 2:C:893:ALA:HB1  | 2:C:897:LEU:CD1   | 2.49                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:945:ARG:HB2   | 2:C:945:ARG:HE    | 1.63                     | 0.43              |
| 3:D:1399:ASP:O    | 3:D:1408:ILE:CD1  | 2.66                     | 0.43              |
| 3:D:1439:SER:OG   | 3:D:1463:LYS:HE2  | 2.18                     | 0.43              |
| 3:D:206:ARG:HG3   | 3:D:393:ILE:HA    | 1.99                     | 0.43              |
| 3:D:238:PRO:CG    | 3:D:318:ARG:HA    | 2.49                     | 0.43              |
| 3:D:570:GLU:O     | 3:D:571:LYS:C     | 2.57                     | 0.43              |
| 3:D:62:LYS:HE3    | 3:D:75:ARG:CZ     | 2.49                     | 0.43              |
| 3:D:806:PHE:CE1   | 3:D:816:HIS:NE2   | 2.87                     | 0.43              |
| 3:D:846:PRO:O     | 3:D:849:ALA:N     | 2.52                     | 0.43              |
| 3:D:930:LEU:HG    | 3:D:934:LEU:CD1   | 2.36                     | 0.43              |
| 5:F:114:LYS:O     | 5:F:115:LYS:C     | 2.55                     | 0.43              |
| 1:K:214:ALA:O     | 1:K:217:ILE:HB    | 2.19                     | 0.43              |
| 2:M:1089:VAL:HG13 | 2:M:1099:VAL:HB   | 2.01                     | 0.43              |
| 2:M:205:GLU:N     | 2:M:209:ARG:NH1   | 2.66                     | 0.43              |
| 2:M:271:GLU:HA    | 2:M:274:ARG:HB3   | 2.00                     | 0.43              |
| 2:M:327:HIS:CE1   | 2:M:433:THR:HG21  | 2.52                     | 0.43              |
| 2:M:100:LEU:CD2   | 2:M:368:THR:HA    | 2.48                     | 0.43              |
| 2:M:439:CYS:CB    | 2:M:541:SER:H     | 2.31                     | 0.43              |
| 2:M:843:HIS:CE1   | 2:M:884:GLN:HA    | 2.54                     | 0.43              |
| 2:M:904:PRO:HD2   | 2:M:908:GLY:HA2   | 1.97                     | 0.43              |
| 2:M:76:PRO:HA     | 2:M:91:GLN:O      | 2.19                     | 0.43              |
| 3:N:1024:ALA:HB2  | 3:N:1035:ILE:HD11 | 1.99                     | 0.43              |
| 3:N:1130:ARG:HH22 | 3:N:1319:VAL:HG12 | 1.84                     | 0.43              |
| 3:N:1332:PRO:O    | 3:N:1333:HIS:C    | 2.56                     | 0.43              |
| 3:N:1341:PRO:C    | 3:N:1345:GLU:HG3  | 2.39                     | 0.43              |
| 3:N:1499:ARG:HD2  | 3:N:1499:ARG:C    | 2.39                     | 0.43              |
| 3:N:178:LEU:HG    | 3:N:181:ASP:CB    | 2.44                     | 0.43              |
| 3:N:197:SER:C     | 3:N:199:LEU:N     | 2.71                     | 0.43              |
| 3:N:41:ARG:HA     | 3:N:46:ASP:OD1    | 2.18                     | 0.43              |
| 3:N:502:PHE:CZ    | 3:N:1452:ILE:HD12 | 2.53                     | 0.43              |
| 3:N:525:ARG:NH1   | 3:N:525:ARG:CG    | 2.78                     | 0.43              |
| 3:N:606:ILE:HG22  | 3:N:607:LEU:N     | 2.33                     | 0.43              |
| 3:N:665:GLY:O     | 3:N:667:ALA:N     | 2.51                     | 0.43              |
| 3:N:45:PHE:O      | 3:N:86:ARG:NH2    | 2.52                     | 0.43              |
| 3:N:891:GLU:HB2   | 3:N:926:LYS:HZ3   | 1.83                     | 0.43              |
| 3:N:972:LEU:N     | 3:N:972:LEU:CD2   | 2.81                     | 0.43              |
| 5:P:188:ILE:HG13  | 5:P:188:ILE:H     | 1.61                     | 0.43              |
| 3:N:566:ILE:CG2   | 5:P:192:LEU:HD22  | 2.48                     | 0.43              |
| 5:P:288:TYR:O     | 5:P:289:GLU:C     | 2.56                     | 0.43              |
| 5:P:347:GLN:O     | 5:P:350:LEU:HB3   | 2.18                     | 0.43              |
| 1:B:104:GLU:HB2   | 1:B:105:GLY:H     | 1.71                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:1052:MET:SD  | 3:D:623:VAL:CG2   | 3.07                     | 0.43              |
| 2:C:383:ARG:O    | 2:C:384:GLU:C     | 2.57                     | 0.43              |
| 2:C:631:SER:HB2  | 2:C:635:THR:OG1   | 2.19                     | 0.43              |
| 2:C:724:ARG:HD2  | 2:C:738:ASP:HA    | 2.01                     | 0.43              |
| 2:C:76:PRO:O     | 2:C:77:PRO:C      | 2.56                     | 0.43              |
| 2:C:832:LYS:CG   | 2:C:833:LEU:N     | 2.82                     | 0.43              |
| 3:D:1069:GLU:HA  | 3:D:1072:ILE:HD12 | 2.00                     | 0.43              |
| 3:D:1262:LEU:O   | 3:D:1264:GLU:N    | 2.52                     | 0.43              |
| 3:D:1379:VAL:HA  | 3:D:1420:LEU:CG   | 2.49                     | 0.43              |
| 3:D:185:VAL:CG2  | 3:D:203:ALA:N     | 2.82                     | 0.43              |
| 3:D:414:ARG:HB3  | 3:D:451:ASP:OD1   | 2.18                     | 0.43              |
| 3:D:452:ILE:HG13 | 3:D:452:ILE:O     | 2.18                     | 0.43              |
| 3:D:491:LYS:O    | 3:D:492:ALA:C     | 2.57                     | 0.43              |
| 3:D:631:ILE:HG21 | 3:D:745:MET:CG    | 2.35                     | 0.43              |
| 3:D:93:ILE:HD13  | 3:D:548:ILE:HG12  | 2.01                     | 0.43              |
| 3:D:945:SER:HG   | 3:D:947:ILE:HG22  | 1.81                     | 0.43              |
| 3:D:965:GLU:HA   | 3:D:965:GLU:OE1   | 2.19                     | 0.43              |
| 4:E:6:ILE:HG13   | 4:E:10:PHE:HE1    | 1.76                     | 0.43              |
| 5:F:110:MET:O    | 5:F:111:GLU:C     | 2.57                     | 0.43              |
| 5:F:109:GLY:O    | 5:F:113:ILE:HG13  | 2.19                     | 0.43              |
| 5:F:144:ILE:C    | 5:F:146:GLY:H     | 2.21                     | 0.43              |
| 3:D:410:SER:OG   | 5:F:164:LYS:HE2   | 2.18                     | 0.43              |
| 5:F:234:LYS:CD   | 5:F:236:SER:HB3   | 2.49                     | 0.43              |
| 5:F:367:MET:CB   | 5:F:370:LYS:HE2   | 2.49                     | 0.43              |
| 5:F:85:LEU:C     | 5:F:87:GLU:N      | 2.71                     | 0.43              |
| 2:M:1014:SER:O   | 2:M:1018:GLN:HA   | 2.19                     | 0.43              |
| 2:M:1068:GLU:O   | 2:M:1071:ILE:HB   | 2.18                     | 0.43              |
| 2:M:276:LYS:HA   | 2:M:280:LYS:HE3   | 2.00                     | 0.43              |
| 2:M:734:LEU:O    | 2:M:735:ARG:C     | 2.57                     | 0.43              |
| 2:M:937:ASP:HB3  | 2:M:940:GLU:HG3   | 1.99                     | 0.43              |
| 2:M:958:THR:O    | 2:M:959:PRO:C     | 2.57                     | 0.43              |
| 3:N:10:ILE:HD13  | 3:N:1450:ALA:HB3  | 2.01                     | 0.43              |
| 3:N:362:GLU:O    | 3:N:363:ALA:C     | 2.57                     | 0.43              |
| 3:N:434:ARG:NH2  | 3:N:451:ASP:OD1   | 2.51                     | 0.43              |
| 3:N:580:ALA:O    | 3:N:584:ASN:HB2   | 2.19                     | 0.43              |
| 5:P:373:LYS:NZ   | 5:P:373:LYS:CB    | 2.72                     | 0.43              |
| 3:N:569:ASN:HB2  | 5:P:84:TYR:CD1    | 2.53                     | 0.43              |
| 1:A:11:PHE:HE2   | 1:B:228:PRO:HA    | 1.84                     | 0.43              |
| 1:A:218:LEU:O    | 1:A:222:LEU:HG    | 2.18                     | 0.43              |
| 1:B:5:LYS:CD     | 1:B:7:LYS:HD2     | 2.45                     | 0.43              |
| 2:C:151:ASP:HA   | 2:C:159:ILE:HG12  | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:176:VAL:HA   | 2:C:183:SER:OG   | 2.18                     | 0.43              |
| 2:C:311:PHE:C    | 2:C:313:LEU:N    | 2.72                     | 0.43              |
| 2:C:326:ASP:HB2  | 2:C:431:HIS:HD2  | 1.83                     | 0.43              |
| 2:C:494:TYR:N    | 2:C:494:TYR:CD1  | 2.87                     | 0.43              |
| 2:C:517:ARG:O    | 2:C:520:GLU:HB2  | 2.18                     | 0.43              |
| 2:C:401:LEU:HD21 | 2:C:543:ASN:HB3  | 2.00                     | 0.43              |
| 2:C:594:ALA:HB1  | 2:C:654:LEU:HD13 | 2.00                     | 0.43              |
| 2:C:873:PRO:HB3  | 3:D:949:ILE:HD12 | 2.00                     | 0.43              |
| 3:D:1001:GLU:O   | 3:D:1002:LYS:C   | 2.57                     | 0.43              |
| 3:D:109:PRO:HB2  | 3:D:114:THR:CB   | 2.48                     | 0.43              |
| 3:D:1397:LYS:O   | 3:D:1401:GLU:OE2 | 2.36                     | 0.43              |
| 3:D:325:GLU:HG3  | 3:D:325:GLU:O    | 2.18                     | 0.43              |
| 3:D:497:GLU:O    | 3:D:498:VAL:C    | 2.57                     | 0.43              |
| 3:D:623:VAL:HG12 | 3:D:624:ASP:N    | 2.34                     | 0.43              |
| 3:D:692:GLU:CD   | 3:D:692:GLU:C    | 2.78                     | 0.43              |
| 3:D:958:GLU:C    | 3:D:960:LYS:N    | 2.72                     | 0.43              |
| 4:E:46:PRO:O     | 4:E:56:ASP:HA    | 2.19                     | 0.43              |
| 5:F:112:ALA:O    | 5:F:115:LYS:N    | 2.52                     | 0.43              |
| 5:F:295:MET:HB3  | 5:F:299:TRP:CG   | 2.53                     | 0.43              |
| 5:F:288:TYR:CB   | 5:F:301:ALA:HB1  | 2.48                     | 0.43              |
| 1:L:178:ALA:O    | 1:L:197:LEU:HD12 | 2.19                     | 0.43              |
| 1:L:19:GLU:O     | 1:L:201:THR:N    | 2.45                     | 0.43              |
| 2:M:1051:GLU:O   | 2:M:1052:MET:C   | 2.57                     | 0.43              |
| 2:M:185:LYS:NZ   | 2:M:190:LYS:HZ3  | 2.17                     | 0.43              |
| 2:M:221:LEU:HD23 | 2:M:221:LEU:C    | 2.39                     | 0.43              |
| 2:M:44:ILE:HG22  | 2:M:48:PHE:CE1   | 2.53                     | 0.43              |
| 2:M:486:MET:SD   | 2:M:490:GLU:HB2  | 2.59                     | 0.43              |
| 2:M:59:LYS:N     | 2:M:59:LYS:CD    | 2.63                     | 0.43              |
| 2:M:692:GLU:HA   | 2:M:852:ILE:CG2  | 2.49                     | 0.43              |
| 3:N:1136:LYS:O   | 3:N:1137:ARG:C   | 2.57                     | 0.43              |
| 3:N:1118:ILE:CG2 | 3:N:1190:SER:HB3 | 2.49                     | 0.43              |
| 3:N:1357:ARG:O   | 3:N:1360:GLY:N   | 2.49                     | 0.43              |
| 3:N:15:PRO:HB2   | 3:N:16:GLU:OE1   | 2.17                     | 0.43              |
| 3:N:256:GLU:HB2  | 3:N:257:GLY:H    | 1.59                     | 0.43              |
| 3:N:545:ARG:O    | 3:N:546:ARG:C    | 2.57                     | 0.43              |
| 3:N:623:VAL:HG13 | 3:N:624:ASP:H    | 1.83                     | 0.43              |
| 2:M:1005:MET:CE  | 3:N:648:MET:HB2  | 2.49                     | 0.43              |
| 3:N:698:LYS:HA   | 3:N:756:GLN:OE1  | 2.19                     | 0.43              |
| 3:N:799:LYS:N    | 3:N:829:VAL:CG1  | 2.82                     | 0.43              |
| 4:O:17:TYR:O     | 4:O:18:ARG:C     | 2.57                     | 0.43              |
| 4:O:66:LYS:HA    | 4:O:66:LYS:HD3   | 1.75                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:163:LEU:N     | 5:P:163:LEU:HD23 | 2.32                     | 0.43              |
| 5:P:191:ASN:O     | 5:P:194:LEU:N    | 2.52                     | 0.43              |
| 5:P:189:GLU:HA    | 5:P:192:LEU:CD1  | 2.49                     | 0.43              |
| 5:P:355:GLU:CA    | 5:P:358:LEU:HB3  | 2.49                     | 0.43              |
| 5:P:381:HIS:O     | 5:P:384:GLU:N    | 2.38                     | 0.43              |
| 5:P:385:GLU:HB2   | 5:P:397:ILE:HD13 | 2.00                     | 0.43              |
| 5:P:79:ASP:O      | 5:P:80:PRO:C     | 2.56                     | 0.43              |
| 1:A:221:HIS:C     | 1:A:223:THR:N    | 2.69                     | 0.43              |
| 1:B:185:ARG:HH22  | 3:D:692:GLU:CG   | 2.23                     | 0.43              |
| 2:C:1090:LYS:HD2  | 3:D:90:MET:SD    | 2.58                     | 0.43              |
| 2:C:1114:GLY:C    | 2:C:1116:ALA:N   | 2.72                     | 0.43              |
| 2:C:273:GLY:O     | 2:C:277:ALA:N    | 2.52                     | 0.43              |
| 2:C:334:ARG:O     | 2:C:339:LEU:HD11 | 2.19                     | 0.43              |
| 2:C:48:PHE:C      | 2:C:50:GLU:H     | 2.22                     | 0.43              |
| 2:C:695:LEU:O     | 2:C:696:LYS:C    | 2.56                     | 0.43              |
| 2:C:882:LEU:O     | 2:C:885:ILE:HB   | 2.19                     | 0.43              |
| 3:D:1353:GLN:C    | 3:D:1355:VAL:N   | 2.70                     | 0.43              |
| 3:D:1397:LYS:N    | 3:D:1398:TRP:HE3 | 2.17                     | 0.43              |
| 3:D:249:TYR:HD2   | 3:D:288:MET:CE   | 2.31                     | 0.43              |
| 3:D:344:ASP:OD1   | 3:D:345:TYR:N    | 2.52                     | 0.43              |
| 3:D:817:GLU:O     | 3:D:821:VAL:HG23 | 2.19                     | 0.43              |
| 3:D:837:GLY:C     | 3:D:839:LEU:N    | 2.72                     | 0.43              |
| 5:F:207:LEU:CB    | 5:F:212:LEU:HD21 | 2.40                     | 0.43              |
| 5:F:379:ARG:C     | 5:F:379:ARG:CD   | 2.87                     | 0.43              |
| 5:F:383:LEU:HD21  | 5:F:394:ARG:HD3  | 2.00                     | 0.43              |
| 2:M:114:PHE:CE2   | 5:P:283:GLY:HA3  | 2.54                     | 0.43              |
| 2:M:159:ILE:HG22  | 2:M:175:GLU:HB2  | 2.01                     | 0.43              |
| 2:M:208:ALA:HB1   | 2:M:222:MET:CG   | 2.49                     | 0.43              |
| 2:M:334:ARG:NH2   | 2:M:342:ASP:OD2  | 2.52                     | 0.43              |
| 2:M:443:THR:OG1   | 2:M:444:PRO:CD   | 2.61                     | 0.43              |
| 2:M:472:ARG:NH2   | 2:M:479:VAL:HG12 | 2.34                     | 0.43              |
| 2:M:495:THR:HB    | 2:M:530:GLU:CG   | 2.48                     | 0.43              |
| 2:M:526:PRO:O     | 2:M:527:GLU:C    | 2.57                     | 0.43              |
| 2:M:860:HIS:HA    | 2:M:866:PRO:HA   | 2.01                     | 0.43              |
| 2:M:889:HIS:O     | 2:M:892:LEU:HB3  | 2.18                     | 0.43              |
| 2:M:918:LEU:HD12  | 2:M:968:LEU:C    | 2.39                     | 0.43              |
| 3:N:1164:ARG:HH21 | 3:N:1170:ASP:CG  | 2.22                     | 0.43              |
| 3:N:1118:ILE:HG12 | 3:N:1190:SER:HB2 | 2.01                     | 0.43              |
| 2:M:1085:PHE:HB2  | 3:N:1468:LEU:O   | 2.19                     | 0.43              |
| 3:N:28:LYS:HA     | 3:N:29:PRO:HD3   | 1.74                     | 0.43              |
| 3:N:138:LYS:CB    | 3:N:450:TYR:OH   | 2.54                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:601:ARG:NH1  | 3:N:601:ARG:HG2  | 2.33                     | 0.43              |
| 3:N:61:GLY:O     | 3:N:62:LYS:C     | 2.56                     | 0.43              |
| 3:N:655:PRO:O    | 3:N:656:PHE:C    | 2.57                     | 0.43              |
| 3:N:671:LYS:HE2  | 3:N:675:ARG:CD   | 2.47                     | 0.43              |
| 3:N:758:GLU:O    | 3:N:762:GLN:HG2  | 2.18                     | 0.43              |
| 3:N:826:PRO:HB3  | 3:N:828:LYS:HZ3  | 1.83                     | 0.43              |
| 3:N:845:ASN:HB3  | 3:N:847:ASP:OD1  | 2.19                     | 0.43              |
| 3:N:845:ASN:N    | 3:N:848:GLU:OE1  | 2.40                     | 0.43              |
| 5:P:102:LEU:HD11 | 5:P:183:ALA:HB1  | 1.95                     | 0.43              |
| 5:P:372:ARG:HA   | 5:P:372:ARG:HD2  | 1.77                     | 0.43              |
| 5:P:380:GLU:C    | 5:P:382:THR:H    | 2.21                     | 0.43              |
| 1:B:211:LEU:O    | 1:B:215:VAL:HG13 | 2.18                     | 0.43              |
| 2:C:1012:PRO:HD3 | 2:C:1026:GLN:CG  | 2.41                     | 0.43              |
| 2:C:1101:THR:OG1 | 2:C:1109:VAL:O   | 2.34                     | 0.43              |
| 2:C:111:ASP:O    | 2:C:112:GLU:HG2  | 2.19                     | 0.43              |
| 2:C:128:ILE:C    | 2:C:129:ILE:HD13 | 2.39                     | 0.43              |
| 2:C:157:ARG:HD3  | 2:C:158:TYR:CZ   | 2.54                     | 0.43              |
| 2:C:170:PRO:HD2  | 2:C:263:ASP:O    | 2.19                     | 0.43              |
| 2:C:247:PRO:HA   | 2:C:248:PRO:HD3  | 1.87                     | 0.43              |
| 2:C:346:VAL:HB   | 2:C:350:ARG:CZ   | 2.49                     | 0.43              |
| 2:C:640:ARG:O    | 2:C:656:ALA:HA   | 2.19                     | 0.43              |
| 3:D:128:TYR:O    | 3:D:129:PHE:C    | 2.55                     | 0.43              |
| 3:D:168:THR:HB   | 3:D:206:ARG:HH12 | 1.84                     | 0.43              |
| 3:D:469:ASP:O    | 3:D:472:ALA:HB3  | 2.19                     | 0.43              |
| 3:D:523:ASP:C    | 3:D:526:PRO:HG3  | 2.38                     | 0.43              |
| 3:D:550:ARG:NH1  | 3:D:573:MET:O    | 2.52                     | 0.43              |
| 3:D:64:LYS:CD    | 5:F:377:ASP:OD2  | 2.67                     | 0.43              |
| 3:D:780:LYS:HB2  | 3:D:781:PRO:HD2  | 2.01                     | 0.43              |
| 5:F:104:ARG:HG3  | 5:F:105:LYS:H    | 1.82                     | 0.43              |
| 5:F:170:HIS:HA   | 5:F:173:TYR:HD1  | 1.84                     | 0.43              |
| 5:F:239:ALA:O    | 5:F:240:THR:C    | 2.56                     | 0.43              |
| 5:F:256:ARG:NH2  | 5:F:310:ILE:O    | 2.52                     | 0.43              |
| 5:F:394:ARG:O    | 5:F:397:ILE:HB   | 2.19                     | 0.43              |
| 1:K:106:PRO:HD3  | 1:K:134:GLU:HA   | 2.00                     | 0.43              |
| 1:K:33:GLY:HA3   | 1:K:181:VAL:CG2  | 2.46                     | 0.43              |
| 1:K:48:ILE:HA    | 1:K:49:PRO:HD3   | 1.85                     | 0.43              |
| 2:M:185:LYS:HZ3  | 2:M:190:LYS:HZ3  | 1.66                     | 0.43              |
| 2:M:196:LEU:HD23 | 2:M:196:LEU:N    | 2.33                     | 0.43              |
| 2:M:208:ALA:CB   | 2:M:221:LEU:HD22 | 2.42                     | 0.43              |
| 2:M:276:LYS:O    | 2:M:277:ALA:C    | 2.56                     | 0.43              |
| 2:M:305:PRO:O    | 2:M:309:TYR:N    | 2.52                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:522:VAL:HG12  | 2:M:523:ILE:H     | 1.83                     | 0.43              |
| 2:M:737:LEU:HD21  | 2:M:741:GLY:O     | 2.18                     | 0.43              |
| 3:N:1111:ASP:OD2  | 3:N:1203:LYS:HG3  | 2.19                     | 0.43              |
| 3:N:1424:VAL:CG2  | 3:N:1425:THR:H    | 2.26                     | 0.43              |
| 3:N:1462:LEU:HD22 | 3:N:1472:ILE:HD12 | 2.01                     | 0.43              |
| 3:N:191:LEU:HD11  | 3:N:393:ILE:HD12  | 2.01                     | 0.43              |
| 3:N:287:GLY:CA    | 3:N:311:LEU:HD22  | 2.49                     | 0.43              |
| 3:N:227:LEU:HB2   | 3:N:329:GLU:O     | 2.18                     | 0.43              |
| 3:N:406:ASP:HB2   | 3:N:423:ASP:CA    | 2.44                     | 0.43              |
| 3:N:894:LYS:HB3   | 3:N:898:GLU:OE1   | 2.18                     | 0.43              |
| 5:P:278:LEU:O     | 5:P:282:LEU:N     | 2.31                     | 0.43              |
| 5:P:348:SER:O     | 5:P:352:GLU:OE2   | 2.36                     | 0.43              |
| 5:P:373:LYS:C     | 5:P:373:LYS:HD2   | 2.38                     | 0.43              |
| 5:P:84:TYR:C      | 5:P:86:HIS:N      | 2.69                     | 0.43              |
| 2:C:157:ARG:CD    | 2:C:314:THR:HG22  | 2.38                     | 0.42              |
| 2:C:352:ALA:C     | 2:C:355:VAL:HG12  | 2.38                     | 0.42              |
| 2:C:615:TYR:O     | 2:C:616:GLU:C     | 2.57                     | 0.42              |
| 2:C:716:LYS:C     | 2:C:718:GLY:H     | 2.21                     | 0.42              |
| 3:D:1126:ASP:O    | 3:D:1126:ASP:OD1  | 2.37                     | 0.42              |
| 3:D:1159:ARG:HG2  | 3:D:1159:ARG:H    | 1.63                     | 0.42              |
| 3:D:1395:LEU:O    | 3:D:1398:TRP:CE3  | 2.72                     | 0.42              |
| 3:D:22:SER:HB2    | 3:D:24:GLY:O      | 2.18                     | 0.42              |
| 3:D:394:LEU:HD12  | 3:D:395:VAL:H     | 1.83                     | 0.42              |
| 3:D:566:ILE:HA    | 3:D:569:ASN:HD22  | 1.83                     | 0.42              |
| 3:D:639:LEU:HG    | 3:D:766:ALA:HB2   | 1.99                     | 0.42              |
| 3:D:661:MET:HB3   | 3:D:667:ALA:CB    | 2.49                     | 0.42              |
| 3:D:796:ARG:HG3   | 3:D:861:GLN:HB3   | 2.00                     | 0.42              |
| 3:D:867:ARG:HA    | 3:D:871:LYS:O     | 2.19                     | 0.42              |
| 4:E:25:LYS:CA     | 4:E:28:GLN:NE2    | 2.78                     | 0.42              |
| 5:F:264:MET:O     | 5:F:267:THR:OG1   | 2.31                     | 0.42              |
| 5:F:394:ARG:HA    | 5:F:397:ILE:HD12  | 2.00                     | 0.42              |
| 1:K:219:ARG:NH1   | 1:K:219:ARG:HG2   | 2.33                     | 0.42              |
| 1:L:209:GLU:H     | 1:L:209:GLU:HG3   | 1.58                     | 0.42              |
| 2:M:240:THR:C     | 2:M:242:LEU:H     | 2.22                     | 0.42              |
| 2:M:27:ARG:C      | 2:M:29:ALA:N      | 2.72                     | 0.42              |
| 2:M:380:ALA:HB1   | 2:M:384:GLU:CG    | 2.49                     | 0.42              |
| 2:M:737:LEU:HD21  | 2:M:741:GLY:C     | 2.39                     | 0.42              |
| 2:M:773:LEU:O     | 2:M:774:LEU:C     | 2.56                     | 0.42              |
| 3:N:119:SER:N     | 3:N:123:LEU:CG    | 2.65                     | 0.42              |
| 3:N:1401:GLU:N    | 3:N:1401:GLU:CD   | 2.72                     | 0.42              |
| 3:N:241:ILE:HG22  | 3:N:242:LEU:N     | 2.34                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:217:LYS:HE3  | 3:N:341:GLU:CD    | 2.39                     | 0.42              |
| 3:N:729:HIS:O    | 3:N:732:VAL:HG22  | 2.19                     | 0.42              |
| 3:N:702:LEU:O    | 3:N:736:PHE:CZ    | 2.71                     | 0.42              |
| 3:N:759:ALA:HA   | 3:N:763:MET:CG    | 2.49                     | 0.42              |
| 3:N:784:ASP:O    | 3:N:785:ILE:C     | 2.57                     | 0.42              |
| 4:O:85:LEU:O     | 4:O:86:GLN:C      | 2.57                     | 0.42              |
| 5:P:207:LEU:HG   | 5:P:211:ASP:HB2   | 2.00                     | 0.42              |
| 5:P:248:ASN:O    | 5:P:249:ARG:C     | 2.57                     | 0.42              |
| 5:P:321:ILE:C    | 5:P:323:ASP:N     | 2.73                     | 0.42              |
| 5:P:356:LYS:HB3  | 5:P:417:LYS:NZ    | 2.33                     | 0.42              |
| 5:P:418:LEU:O    | 5:P:419:ARG:C     | 2.57                     | 0.42              |
| 1:B:118:ALA:C    | 1:B:120:VAL:H     | 2.22                     | 0.42              |
| 1:B:61:VAL:CG2   | 1:B:62:LEU:N      | 2.82                     | 0.42              |
| 2:C:1071:ILE:C   | 2:C:1073:GLY:N    | 2.71                     | 0.42              |
| 2:C:202:TYR:HB2  | 2:C:207:LEU:CD1   | 2.47                     | 0.42              |
| 2:C:23:VAL:CG2   | 2:C:24:GLU:N      | 2.82                     | 0.42              |
| 2:C:260:LEU:HB2  | 2:C:291:ALA:CB    | 2.49                     | 0.42              |
| 2:C:432:ARG:HG3  | 2:C:433:THR:N     | 2.34                     | 0.42              |
| 2:C:589:ARG:NH2  | 2:C:652:GLY:O     | 2.52                     | 0.42              |
| 2:C:605:LYS:HB3  | 2:C:610:ARG:HH22  | 1.80                     | 0.42              |
| 2:C:910:LYS:N    | 2:C:913:GLU:OE1   | 2.52                     | 0.42              |
| 3:D:1012:GLU:O   | 3:D:1016:PRO:HG3  | 2.19                     | 0.42              |
| 3:D:1071:PHE:O   | 3:D:1072:ILE:C    | 2.58                     | 0.42              |
| 3:D:1143:GLY:HA2 | 3:D:1365:ASP:OD1  | 2.20                     | 0.42              |
| 3:D:117:ASP:HB2  | 3:D:495:ARG:NH1   | 2.34                     | 0.42              |
| 3:D:119:SER:H    | 3:D:123:LEU:HB2   | 1.83                     | 0.42              |
| 3:D:1232:PRO:HB2 | 3:D:1356:TYR:CE2  | 2.54                     | 0.42              |
| 3:D:125:GLN:O    | 3:D:126:VAL:C     | 2.57                     | 0.42              |
| 3:D:1380:GLU:HB2 | 3:D:1420:LEU:HD11 | 2.01                     | 0.42              |
| 3:D:206:ARG:HB3  | 3:D:207:PHE:HD1   | 1.83                     | 0.42              |
| 3:D:269:PHE:HD1  | 3:D:283:PHE:CB    | 2.28                     | 0.42              |
| 3:D:608:SER:O    | 3:D:609:GLY:C     | 2.57                     | 0.42              |
| 3:D:710:ARG:C    | 3:D:712:GLY:N     | 2.73                     | 0.42              |
| 3:D:632:VAL:N    | 3:D:726:ILE:O     | 2.46                     | 0.42              |
| 3:D:60:CYS:SG    | 3:D:76:CYS:CB     | 3.04                     | 0.42              |
| 3:D:829:VAL:HB   | 3:D:830:ALA:H     | 1.69                     | 0.42              |
| 3:D:87:ARG:HG3   | 3:D:88:TYR:CE2    | 2.54                     | 0.42              |
| 3:D:886:VAL:O    | 3:D:890:VAL:HG22  | 2.19                     | 0.42              |
| 3:D:915:VAL:O    | 3:D:916:TYR:C     | 2.57                     | 0.42              |
| 4:E:26:ARG:O     | 4:E:29:GLN:HG2    | 2.20                     | 0.42              |
| 5:F:183:ALA:O    | 5:F:184:ARG:C     | 2.58                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:31:THR:OG1   | 5:F:258:ILE:HD13 | 2.19                     | 0.42              |
| 5:F:300:ASP:OD2  | 5:F:302:LYS:HE3  | 2.20                     | 0.42              |
| 5:F:321:ILE:O    | 5:F:323:ASP:N    | 2.52                     | 0.42              |
| 5:F:79:ASP:HB2   | 5:F:81:VAL:HG22  | 2.01                     | 0.42              |
| 5:F:99:GLU:O     | 5:F:100:VAL:C    | 2.58                     | 0.42              |
| 1:K:40:LEU:O     | 1:K:43:ILE:N     | 2.52                     | 0.42              |
| 1:L:112:ARG:HH11 | 1:L:112:ARG:CB   | 2.31                     | 0.42              |
| 2:M:1060:ILE:O   | 2:M:1061:GLU:C   | 2.57                     | 0.42              |
| 2:M:1107:ASN:HA  | 2:M:1108:PRO:HD3 | 1.91                     | 0.42              |
| 2:M:151:ASP:CB   | 2:M:157:ARG:O    | 2.64                     | 0.42              |
| 2:M:182:VAL:HG21 | 2:M:194:VAL:CG2  | 2.49                     | 0.42              |
| 2:M:198:ARG:CG   | 2:M:228:ALA:HA   | 2.49                     | 0.42              |
| 2:M:20:GLU:O     | 2:M:23:VAL:HG23  | 2.18                     | 0.42              |
| 2:M:289:THR:HG22 | 2:M:290:LEU:HD21 | 2.00                     | 0.42              |
| 2:M:341:THR:O    | 2:M:344:PHE:N    | 2.51                     | 0.42              |
| 2:M:537:LYS:HG3  | 2:M:537:LYS:H    | 1.36                     | 0.42              |
| 2:M:562:SER:O    | 2:M:564:MET:N    | 2.51                     | 0.42              |
| 2:M:583:LEU:O    | 2:M:584:GLU:C    | 2.56                     | 0.42              |
| 2:M:731:GLU:C    | 2:M:733:ALA:N    | 2.73                     | 0.42              |
| 2:M:731:GLU:HA   | 2:M:734:LEU:CD1  | 2.49                     | 0.42              |
| 3:N:1003:VAL:O   | 3:N:1004:THR:C   | 2.57                     | 0.42              |
| 3:N:119:SER:CA   | 3:N:123:LEU:HG   | 2.48                     | 0.42              |
| 3:N:1417:TRP:CD1 | 3:N:1418:LYS:N   | 2.88                     | 0.42              |
| 3:N:1496:GLU:OE1 | 3:N:1499:ARG:NE  | 2.52                     | 0.42              |
| 3:N:262:LYS:HG2  | 3:N:263:GLU:N    | 2.34                     | 0.42              |
| 3:N:591:VAL:HB   | 3:N:598:ARG:O    | 2.20                     | 0.42              |
| 3:N:749:VAL:HA   | 3:N:750:PRO:HD2  | 1.93                     | 0.42              |
| 3:N:826:PRO:CD   | 3:N:829:VAL:HG11 | 2.37                     | 0.42              |
| 3:N:1489:GLN:NE2 | 4:O:71:GLY:O     | 2.39                     | 0.42              |
| 5:P:236:SER:C    | 5:P:238:TYR:N    | 2.72                     | 0.42              |
| 5:P:287:THR:HG23 | 5:P:290:GLU:CD   | 2.38                     | 0.42              |
| 5:P:300:ASP:HB3  | 5:P:302:LYS:NZ   | 2.34                     | 0.42              |
| 5:P:330:GLY:C    | 5:P:332:PHE:N    | 2.70                     | 0.42              |
| 1:A:184:THR:O    | 1:A:192:LEU:HB2  | 2.19                     | 0.42              |
| 1:B:55:SER:O     | 1:B:143:ARG:HB3  | 2.19                     | 0.42              |
| 2:C:198:ARG:HD2  | 2:C:198:ARG:HA   | 1.90                     | 0.42              |
| 2:C:204:GLN:HG2  | 2:C:222:MET:HG2  | 2.00                     | 0.42              |
| 2:C:335:THR:O    | 2:C:336:VAL:C    | 2.57                     | 0.42              |
| 2:C:368:THR:CB   | 2:C:369:PRO:CD   | 2.94                     | 0.42              |
| 2:C:460:ARG:O    | 2:C:467:ILE:HA   | 2.19                     | 0.42              |
| 2:C:472:ARG:CZ   | 2:C:479:VAL:HG12 | 2.50                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:701:THR:HA    | 2:C:832:LYS:HA   | 2.01                     | 0.42              |
| 3:D:1496:GLU:CA   | 3:D:1499:ARG:HB3 | 2.47                     | 0.42              |
| 3:D:17:LYS:O      | 3:D:18:ILE:C     | 2.56                     | 0.42              |
| 3:D:227:LEU:HD11  | 3:D:326:GLU:CA   | 2.33                     | 0.42              |
| 3:D:25:GLU:OE2    | 3:D:94:GLU:HB2   | 2.19                     | 0.42              |
| 3:D:210:ARG:HD2   | 3:D:389:GLU:HG3  | 2.00                     | 0.42              |
| 3:D:409:VAL:HB    | 5:F:164:LYS:HZ3  | 1.84                     | 0.42              |
| 3:D:610:LYS:O     | 3:D:612:GLY:N    | 2.46                     | 0.42              |
| 3:D:761:ILE:HD13  | 4:E:20:THR:HA    | 2.01                     | 0.42              |
| 3:D:800:LYS:NZ    | 3:D:825:ALA:HA   | 2.34                     | 0.42              |
| 3:D:828:LYS:H     | 3:D:828:LYS:CE   | 2.32                     | 0.42              |
| 3:D:862:ASP:O     | 3:D:877:PRO:HD3  | 2.19                     | 0.42              |
| 5:F:350:LEU:C     | 5:F:352:GLU:N    | 2.72                     | 0.42              |
| 1:K:221:HIS:C     | 1:K:223:THR:N    | 2.71                     | 0.42              |
| 1:L:94:LEU:O      | 1:L:146:ARG:CZ   | 2.68                     | 0.42              |
| 2:M:193:LEU:HD12  | 2:M:196:LEU:HD12 | 2.01                     | 0.42              |
| 2:M:227:PHE:N     | 2:M:227:PHE:HD1  | 2.16                     | 0.42              |
| 2:M:267:TYR:CD1   | 2:M:272:ALA:HB2  | 2.55                     | 0.42              |
| 2:M:409:ARG:HA    | 2:M:454:SER:HA   | 2.01                     | 0.42              |
| 2:M:563:ASN:O     | 2:M:567:GLN:HG3  | 2.19                     | 0.42              |
| 2:M:58:ASP:C      | 2:M:59:LYS:HD2   | 2.36                     | 0.42              |
| 2:M:928:LYS:HE2   | 2:M:932:GLU:CG   | 2.49                     | 0.42              |
| 2:M:963:LEU:N     | 2:M:963:LEU:HD23 | 2.33                     | 0.42              |
| 3:N:1114:THR:HG23 | 3:N:1114:THR:O   | 2.19                     | 0.42              |
| 3:N:1118:ILE:HD13 | 3:N:1190:SER:CB  | 2.48                     | 0.42              |
| 3:N:1213:ARG:HG2  | 3:N:1213:ARG:NH1 | 2.18                     | 0.42              |
| 3:N:1378:TYR:CZ   | 3:N:1430:SER:HB2 | 2.54                     | 0.42              |
| 3:N:117:ASP:HB2   | 3:N:150:ARG:NH2  | 2.34                     | 0.42              |
| 3:N:211:VAL:HA    | 3:N:387:LEU:HA   | 2.01                     | 0.42              |
| 3:N:259:VAL:C     | 3:N:260:GLU:HG3  | 2.40                     | 0.42              |
| 3:N:331:VAL:HG12  | 3:N:333:LEU:HD23 | 2.00                     | 0.42              |
| 3:N:337:LEU:HD23  | 3:N:337:LEU:N    | 2.34                     | 0.42              |
| 3:N:411:THR:H     | 3:N:437:VAL:HG23 | 1.84                     | 0.42              |
| 3:N:505:SER:HB3   | 3:N:1453:ALA:O   | 2.19                     | 0.42              |
| 3:N:553:ARG:O     | 3:N:554:LEU:C    | 2.58                     | 0.42              |
| 3:N:895:VAL:HA    | 3:N:898:GLU:CD   | 2.40                     | 0.42              |
| 3:N:912:LYS:O     | 3:N:915:VAL:HB   | 2.19                     | 0.42              |
| 3:N:970:LYS:O     | 3:N:973:GLN:N    | 2.52                     | 0.42              |
| 5:P:102:LEU:O     | 5:P:105:LYS:HB2  | 2.18                     | 0.42              |
| 5:P:208:SER:O     | 5:P:209:PHE:C    | 2.58                     | 0.42              |
| 5:P:371:LEU:O     | 5:P:375:LEU:HB3  | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:382:THR:HG21  | 5:P:394:ARG:HB2   | 2.01                     | 0.42              |
| 1:A:63:HIS:CE1    | 1:A:65:PHE:C      | 2.93                     | 0.42              |
| 2:C:1012:PRO:HD2  | 2:C:1021:LEU:O    | 2.19                     | 0.42              |
| 2:C:1052:MET:HA   | 2:C:1056:LYS:HD2  | 2.01                     | 0.42              |
| 2:C:234:ALA:O     | 2:C:238:LEU:HG    | 2.20                     | 0.42              |
| 2:C:276:LYS:O     | 2:C:277:ALA:C     | 2.57                     | 0.42              |
| 2:C:276:LYS:O     | 2:C:280:LYS:HG3   | 2.19                     | 0.42              |
| 2:C:260:LEU:C     | 2:C:288:ARG:NH2   | 2.73                     | 0.42              |
| 2:C:56:GLU:O      | 2:C:359:MET:SD    | 2.77                     | 0.42              |
| 2:C:503:LEU:HD12  | 2:C:508:ILE:CA    | 2.36                     | 0.42              |
| 2:C:474:VAL:HG12  | 2:C:530:GLU:CA    | 2.49                     | 0.42              |
| 2:C:575:GLN:HE21  | 2:C:670:GLN:CG    | 2.32                     | 0.42              |
| 1:A:65:PHE:HA     | 2:C:628:PHE:HE2   | 1.85                     | 0.42              |
| 2:C:644:VAL:O     | 2:C:647:GLN:HB3   | 2.19                     | 0.42              |
| 3:D:1094:LEU:CD1  | 3:D:1098:LEU:HD11 | 2.49                     | 0.42              |
| 3:D:1269:LYS:N    | 3:D:1269:LYS:HD3  | 2.34                     | 0.42              |
| 3:D:1197:ARG:HG3  | 3:D:1396:GLU:OE1  | 2.20                     | 0.42              |
| 3:D:1103:HIS:CD2  | 3:D:1462:LEU:N    | 2.87                     | 0.42              |
| 3:D:18:ILE:HD13   | 3:D:516:ALA:O     | 2.19                     | 0.42              |
| 3:D:28:LYS:HA     | 3:D:29:PRO:HD3    | 1.77                     | 0.42              |
| 3:D:37:LEU:HD23   | 3:D:37:LEU:N      | 2.33                     | 0.42              |
| 3:D:462:GLN:HG2   | 3:D:466:LYS:HE3   | 2.00                     | 0.42              |
| 3:D:528:VAL:C     | 3:D:535:PHE:HB3   | 2.39                     | 0.42              |
| 3:D:596:SER:C     | 3:D:598:ARG:N     | 2.73                     | 0.42              |
| 3:D:704:ARG:NE    | 3:D:738:ALA:HB2   | 2.33                     | 0.42              |
| 3:D:698:LYS:HA    | 3:D:756:GLN:HE22  | 1.83                     | 0.42              |
| 3:D:807:ALA:CB    | 3:D:833:GLU:CD    | 2.87                     | 0.42              |
| 3:D:860:LEU:H     | 3:D:860:LEU:HG    | 1.55                     | 0.42              |
| 4:E:41:GLU:HB2    | 4:E:42:PRO:CD     | 2.37                     | 0.42              |
| 5:F:107:GLU:OE2   | 5:F:229:TYR:HD1   | 2.02                     | 0.42              |
| 5:F:262:VAL:C     | 5:F:264:MET:N     | 2.69                     | 0.42              |
| 2:C:1015:LEU:HD12 | 5:F:335:ASP:HA    | 2.00                     | 0.42              |
| 5:F:414:ARG:HE    | 5:F:414:ARG:N     | 2.17                     | 0.42              |
| 1:K:110:LYS:HA    | 1:K:127:LEU:O     | 2.19                     | 0.42              |
| 1:K:55:SER:HB2    | 1:K:165:ILE:O     | 2.19                     | 0.42              |
| 2:M:1059:ASP:OD1  | 2:M:1080:SER:OG   | 2.37                     | 0.42              |
| 2:M:1084:SER:OG   | 2:M:1085:PHE:N    | 2.52                     | 0.42              |
| 2:M:1098:ASP:CB   | 3:N:17:LYS:NZ     | 2.83                     | 0.42              |
| 2:M:182:VAL:HB    | 2:M:193:LEU:N     | 2.29                     | 0.42              |
| 2:M:182:VAL:CG2   | 2:M:221:LEU:HA    | 2.49                     | 0.42              |
| 2:M:270:GLY:O     | 2:M:271:GLU:C     | 2.57                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:267:TYR:CB    | 2:M:272:ALA:H    | 2.32                     | 0.42              |
| 2:M:612:VAL:HA    | 2:M:622:GLU:HA   | 2.01                     | 0.42              |
| 2:M:588:VAL:HG21  | 2:M:664:GLY:O    | 2.20                     | 0.42              |
| 2:M:874:LEU:HD23  | 3:N:1023:MET:SD  | 2.59                     | 0.42              |
| 3:N:1005:GLN:O    | 3:N:1006:ALA:C   | 2.57                     | 0.42              |
| 3:N:1175:ILE:O    | 3:N:1179:GLU:N   | 2.48                     | 0.42              |
| 3:N:1207:TYR:HA   | 3:N:1214:PRO:HA  | 2.02                     | 0.42              |
| 3:N:1399:ASP:O    | 3:N:1400:VAL:C   | 2.56                     | 0.42              |
| 3:N:1491:THR:HG23 | 3:N:1494:ALA:HB2 | 1.99                     | 0.42              |
| 3:N:446:VAL:O     | 3:N:446:VAL:HG12 | 2.18                     | 0.42              |
| 3:N:455:ARG:HB2   | 3:N:460:ALA:CB   | 2.47                     | 0.42              |
| 3:N:544:TYR:O     | 3:N:547:LEU:N    | 2.52                     | 0.42              |
| 3:N:602:SER:O     | 3:N:605:ASP:HB2  | 2.20                     | 0.42              |
| 3:N:642:CYS:SG    | 3:N:716:PHE:CB   | 3.00                     | 0.42              |
| 3:N:658:LEU:N     | 3:N:661:MET:HE3  | 2.34                     | 0.42              |
| 3:N:670:VAL:O     | 3:N:671:LYS:C    | 2.56                     | 0.42              |
| 3:N:673:ALA:O     | 3:N:677:LEU:HG   | 2.19                     | 0.42              |
| 3:N:909:ASN:HA    | 3:N:912:LYS:HZ2  | 1.85                     | 0.42              |
| 4:O:5:GLY:O       | 4:O:9:LEU:HG     | 2.19                     | 0.42              |
| 5:P:209:PHE:HA    | 5:P:212:LEU:HG   | 2.01                     | 0.42              |
| 5:P:276:ARG:C     | 5:P:278:LEU:N    | 2.73                     | 0.42              |
| 5:P:305:GLU:HA    | 5:P:308:LEU:CD1  | 2.48                     | 0.42              |
| 5:P:354:LEU:O     | 5:P:355:GLU:C    | 2.58                     | 0.42              |
| 5:P:361:LEU:HG    | 5:P:362:SER:H    | 1.83                     | 0.42              |
| 1:A:14:ARG:HH11   | 1:A:14:ARG:HG2   | 1.85                     | 0.42              |
| 1:A:20:TYR:CG     | 1:A:21:GLY:N     | 2.87                     | 0.42              |
| 1:B:217:ILE:O     | 1:B:220:GLU:HB3  | 2.19                     | 0.42              |
| 2:C:1066:ALA:O    | 2:C:1069:ALA:HB3 | 2.20                     | 0.42              |
| 2:C:13:ILE:N      | 2:C:13:ILE:HD13  | 2.33                     | 0.42              |
| 2:C:24:GLU:OE2    | 2:C:27:ARG:HD3   | 2.19                     | 0.42              |
| 2:C:347:GLY:HA2   | 2:C:350:ARG:HB2  | 2.01                     | 0.42              |
| 2:C:569:VAL:HA    | 2:C:570:PRO:HD3  | 1.79                     | 0.42              |
| 2:C:58:ASP:C      | 2:C:60:GLY:N     | 2.73                     | 0.42              |
| 1:A:196:THR:HG21  | 2:C:934:PHE:CE2  | 2.55                     | 0.42              |
| 3:D:957:PRO:CG    | 3:D:1007:VAL:HA  | 2.37                     | 0.42              |
| 3:D:102:ILE:O     | 3:D:105:VAL:N    | 2.51                     | 0.42              |
| 3:D:1128:VAL:HG23 | 3:D:1131:SER:HB3 | 1.91                     | 0.42              |
| 3:D:1169:ASP:O    | 3:D:1170:ASP:C   | 2.57                     | 0.42              |
| 3:D:119:SER:HB3   | 3:D:123:LEU:CG   | 2.43                     | 0.42              |
| 3:D:288:MET:CG    | 3:D:305:ALA:HB1  | 2.50                     | 0.42              |
| 3:D:307:ALA:O     | 3:D:308:LYS:HD3  | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:384:VAL:CG1   | 3:D:385:VAL:N    | 2.82                     | 0.42              |
| 3:D:421:LEU:HB3   | 3:D:427:VAL:C    | 2.40                     | 0.42              |
| 3:D:433:GLY:HA3   | 3:D:447:VAL:O    | 2.19                     | 0.42              |
| 3:D:128:TYR:CD1   | 3:D:457:GLY:CA   | 2.98                     | 0.42              |
| 3:D:542:ASP:CA    | 3:D:545:ARG:HG3  | 2.50                     | 0.42              |
| 3:D:545:ARG:HB2   | 3:D:546:ARG:H    | 1.64                     | 0.42              |
| 3:D:673:ALA:C     | 3:D:676:MET:HB3  | 2.40                     | 0.42              |
| 3:D:807:ALA:H     | 3:D:809:PRO:HD2  | 1.84                     | 0.42              |
| 3:D:808:THR:N     | 3:D:809:PRO:CD   | 2.72                     | 0.42              |
| 3:D:85:VAL:CG2    | 3:D:89:ARG:HG3   | 2.49                     | 0.42              |
| 3:D:85:VAL:HG22   | 3:D:89:ARG:HG3   | 1.99                     | 0.42              |
| 3:D:900:ILE:HG22  | 3:D:901:GLN:N    | 2.34                     | 0.42              |
| 4:E:33:HIS:O      | 4:E:34:GLY:C     | 2.57                     | 0.42              |
| 4:E:88:GLU:HA     | 4:E:91:ARG:HD2   | 2.02                     | 0.42              |
| 5:F:307:THR:O     | 5:F:310:ILE:N    | 2.52                     | 0.42              |
| 1:K:151:VAL:HG12  | 1:K:156:HIS:ND1  | 2.34                     | 0.42              |
| 1:K:167:VAL:HG12  | 1:K:168:ASP:O    | 2.19                     | 0.42              |
| 1:K:185:ARG:HB2   | 1:K:190:THR:HG22 | 2.02                     | 0.42              |
| 1:K:202:ASP:OD1   | 1:K:204:SER:N    | 2.53                     | 0.42              |
| 1:L:10:VAL:O      | 1:L:10:VAL:CG2   | 2.68                     | 0.42              |
| 2:M:144:PRO:O     | 2:M:276:LYS:NZ   | 2.44                     | 0.42              |
| 2:M:205:GLU:CA    | 2:M:209:ARG:HD3  | 2.49                     | 0.42              |
| 2:M:25:SER:O      | 2:M:29:ALA:HB2   | 2.19                     | 0.42              |
| 2:M:558:ALA:O     | 2:M:559:LEU:C    | 2.57                     | 0.42              |
| 2:M:602:GLU:HG2   | 2:M:603:VAL:N    | 2.33                     | 0.42              |
| 2:M:614:ARG:HG3   | 2:M:620:LEU:HD21 | 2.01                     | 0.42              |
| 2:M:602:GLU:CD    | 2:M:646:GLY:HA2  | 2.39                     | 0.42              |
| 2:M:749:VAL:HG23  | 2:M:750:LYS:N    | 2.35                     | 0.42              |
| 2:M:777:ILE:O     | 2:M:777:ILE:HG22 | 2.19                     | 0.42              |
| 2:M:833:LEU:CD1   | 2:M:837:ASP:CB   | 2.98                     | 0.42              |
| 3:N:998:GLU:OE2   | 3:N:1002:LYS:HE3 | 2.19                     | 0.42              |
| 3:N:1071:PHE:O    | 3:N:1072:ILE:C   | 2.58                     | 0.42              |
| 3:N:1155:VAL:HG11 | 3:N:1177:ALA:HB1 | 2.02                     | 0.42              |
| 3:N:1194:CYS:SG   | 3:N:1195:GLN:N   | 2.92                     | 0.42              |
| 3:N:169:TYR:HB3   | 3:N:195:VAL:CG1  | 2.50                     | 0.42              |
| 3:N:819:GLY:CA    | 3:N:824:ASN:ND2  | 2.70                     | 0.42              |
| 3:N:82:LYS:HB2    | 3:N:84:ILE:CG2   | 2.34                     | 0.42              |
| 3:N:887:ALA:HA    | 3:N:890:VAL:CG2  | 2.47                     | 0.42              |
| 4:O:40:LEU:HD13   | 4:O:72:ARG:NH2   | 2.34                     | 0.42              |
| 5:P:96:LEU:O      | 5:P:100:VAL:HG23 | 2.19                     | 0.42              |
| 5:P:135:ILE:C     | 5:P:137:GLY:N    | 2.72                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:215:GLU:OE1   | 5:P:215:GLU:HA    | 2.20                     | 0.42              |
| 5:P:279:GLN:HA    | 5:P:286:PRO:CD    | 2.49                     | 0.42              |
| 5:P:382:THR:HA    | 5:P:385:GLU:HB2   | 2.01                     | 0.42              |
| 1:A:83:LYS:HE3    | 1:A:167:VAL:HG12  | 2.02                     | 0.42              |
| 2:C:121:MET:HG3   | 2:C:127:PHE:CE1   | 2.54                     | 0.42              |
| 2:C:141:HIS:HE1   | 2:C:144:PRO:HD3   | 1.85                     | 0.42              |
| 2:C:177:GLU:HA    | 2:C:178:PRO:HD2   | 1.86                     | 0.42              |
| 2:C:346:VAL:CG2   | 2:C:347:GLY:N     | 2.74                     | 0.42              |
| 2:C:62:GLY:HA3    | 2:C:103:LYS:HB2   | 2.01                     | 0.42              |
| 2:C:930:LYS:O     | 2:C:932:GLU:N     | 2.53                     | 0.42              |
| 2:C:967:PHE:O     | 2:C:970:GLY:N     | 2.50                     | 0.42              |
| 3:D:1078:ARG:C    | 3:D:1080:GLY:N    | 2.72                     | 0.42              |
| 3:D:154:THR:CG2   | 3:D:156:GLU:OE2   | 2.67                     | 0.42              |
| 3:D:15:PRO:HB2    | 3:D:16:GLU:OE1    | 2.20                     | 0.42              |
| 3:D:185:VAL:HA    | 3:D:189:GLN:HE22  | 1.83                     | 0.42              |
| 3:D:470:LEU:O     | 3:D:472:ALA:N     | 2.52                     | 0.42              |
| 3:D:739:ASP:OD1   | 3:D:741:ASP:OD1   | 2.37                     | 0.42              |
| 3:D:924:MET:CG    | 3:D:925:GLU:N     | 2.83                     | 0.42              |
| 5:F:156:VAL:HG23  | 5:F:157:GLU:OE1   | 2.20                     | 0.42              |
| 5:F:365:GLU:O     | 5:F:368:VAL:CG2   | 2.66                     | 0.42              |
| 1:K:100:LEU:CD2   | 1:K:101:LEU:N     | 2.81                     | 0.42              |
| 2:M:1040:LEU:HD13 | 2:M:1049:LEU:CA   | 2.49                     | 0.42              |
| 2:M:1076:VAL:HA   | 2:M:1077:PRO:HD3  | 1.80                     | 0.42              |
| 2:M:121:MET:SD    | 2:M:125:GLY:HA2   | 2.60                     | 0.42              |
| 2:M:191:PHE:HE2   | 2:M:196:LEU:HD21  | 1.81                     | 0.42              |
| 2:M:415:PRO:HG2   | 2:M:418:LEU:HD12  | 2.00                     | 0.42              |
| 2:M:430:VAL:HG23  | 2:M:434:HIS:HD2   | 1.83                     | 0.42              |
| 2:M:479:VAL:N     | 2:M:506:ASN:HB3   | 2.25                     | 0.42              |
| 2:M:494:TYR:O     | 2:M:517:ARG:HA    | 2.20                     | 0.42              |
| 2:M:573:ARG:HB2   | 2:M:670:GLN:HE22  | 1.84                     | 0.42              |
| 2:M:657:ASP:O     | 2:M:658:GLY:O     | 2.37                     | 0.42              |
| 2:M:712:ALA:O     | 2:M:820:ARG:N     | 2.37                     | 0.42              |
| 2:M:762:LYS:HB2   | 2:M:786:LYS:HD2   | 2.02                     | 0.42              |
| 2:M:78:PHE:HD2    | 2:M:82:GLU:OE2    | 2.02                     | 0.42              |
| 2:M:9:ILE:O       | 2:M:10:ARG:C      | 2.57                     | 0.42              |
| 3:N:1025:GLN:C    | 3:N:1027:GLY:N    | 2.73                     | 0.42              |
| 3:N:106:LYS:HB3   | 3:N:586:ARG:CZ    | 2.49                     | 0.42              |
| 3:N:1186:VAL:HA   | 3:N:1187:PRO:HD3  | 1.83                     | 0.42              |
| 3:N:133:ILE:HG13  | 3:N:158:TYR:CG    | 2.54                     | 0.42              |
| 3:N:1385:GLY:HA2  | 3:N:1413:THR:HG21 | 2.00                     | 0.42              |
| 3:N:13:ALA:HA     | 3:N:17:LYS:HD3    | 2.02                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:407:VAL:CG2  | 3:N:408:GLU:N    | 2.63                     | 0.42              |
| 4:O:29:GLN:C     | 4:O:31:LEU:N     | 2.73                     | 0.42              |
| 5:P:214:GLN:HA   | 5:P:214:GLN:OE1  | 2.19                     | 0.42              |
| 5:P:302:LYS:O    | 5:P:306:GLU:HG2  | 2.20                     | 0.42              |
| 5:P:321:ILE:HG13 | 5:P:332:PHE:CZ   | 2.51                     | 0.42              |
| 1:A:31:GLY:O     | 1:A:32:PHE:C     | 2.58                     | 0.42              |
| 1:A:79:ILE:HG13  | 1:A:79:ILE:H     | 1.46                     | 0.42              |
| 1:A:5:LYS:C      | 1:A:7:LYS:H      | 2.21                     | 0.42              |
| 1:B:91:ASN:ND2   | 1:B:91:ASN:C     | 2.72                     | 0.42              |
| 2:C:1114:GLY:O   | 2:C:1116:ALA:N   | 2.52                     | 0.42              |
| 2:C:402:SER:HA   | 2:C:566:THR:HG22 | 2.00                     | 0.42              |
| 2:C:546:LEU:HD23 | 2:C:583:LEU:HD12 | 2.00                     | 0.42              |
| 2:C:649:VAL:CA   | 2:C:650:ARG:HH21 | 2.24                     | 0.42              |
| 2:C:737:LEU:HD11 | 2:C:741:GLY:O    | 2.20                     | 0.42              |
| 2:C:742:VAL:HG12 | 2:C:743:VAL:H    | 1.83                     | 0.42              |
| 3:D:1042:ARG:HG2 | 3:D:1042:ARG:NH1 | 2.32                     | 0.42              |
| 3:D:1191:PRO:O   | 3:D:1192:LEU:C   | 2.58                     | 0.42              |
| 3:D:148:GLU:O    | 3:D:149:LYS:C    | 2.58                     | 0.42              |
| 3:D:168:THR:OG1  | 3:D:206:ARG:NH1  | 2.53                     | 0.42              |
| 3:D:231:VAL:O    | 3:D:231:VAL:HG12 | 2.19                     | 0.42              |
| 3:D:511:TRP:CA   | 3:D:511:TRP:CE3  | 3.02                     | 0.42              |
| 3:D:654:LYS:CB   | 3:D:655:PRO:CD   | 2.97                     | 0.42              |
| 3:D:56:TYR:CE2   | 3:D:66:GLN:HG3   | 2.55                     | 0.42              |
| 2:C:1102:LEU:N   | 3:D:7:LYS:O      | 2.43                     | 0.42              |
| 3:D:854:ALA:C    | 3:D:856:GLY:H    | 2.22                     | 0.42              |
| 5:F:140:ARG:HH11 | 5:F:140:ARG:HG3  | 1.83                     | 0.42              |
| 5:F:196:VAL:C    | 5:F:198:ILE:N    | 2.73                     | 0.42              |
| 5:F:282:LEU:CG   | 5:F:284:ARG:HG2  | 2.36                     | 0.42              |
| 5:F:421:PHE:HD2  | 5:F:422:LEU:N    | 2.17                     | 0.42              |
| 1:L:210:ALA:O    | 1:L:213:GLN:HB2  | 2.18                     | 0.42              |
| 1:L:82:LEU:C     | 1:L:84:GLU:N     | 2.73                     | 0.42              |
| 2:M:164:PRO:HB2  | 2:M:263:ASP:O    | 2.17                     | 0.42              |
| 2:M:18:LEU:HG    | 2:M:590:ASP:CG   | 2.40                     | 0.42              |
| 2:M:401:LEU:O    | 2:M:404:LEU:N    | 2.52                     | 0.42              |
| 2:M:494:TYR:CD1  | 2:M:494:TYR:N    | 2.88                     | 0.42              |
| 2:M:799:ILE:O    | 2:M:827:VAL:HG13 | 2.20                     | 0.42              |
| 2:M:944:LEU:O    | 2:M:945:ARG:C    | 2.58                     | 0.42              |
| 2:M:425:PHE:HZ   | 3:N:1083:ASP:HB2 | 1.85                     | 0.42              |
| 3:N:1272:ALA:HB2 | 3:N:1328:GLY:CA  | 2.50                     | 0.42              |
| 3:N:1342:GLU:N   | 3:N:1342:GLU:OE1 | 2.51                     | 0.42              |
| 3:N:1344:VAL:O   | 3:N:1348:LEU:HG  | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:1424:VAL:CG2 | 3:N:1425:THR:N    | 2.79                     | 0.42              |
| 3:N:187:LYS:HE3  | 3:N:198:ARG:HG3   | 2.02                     | 0.42              |
| 3:N:268:ALA:CB   | 3:N:290:PRO:HG3   | 2.44                     | 0.42              |
| 3:N:47:GLU:C     | 3:N:49:ILE:N      | 2.72                     | 0.42              |
| 3:N:729:HIS:HE1  | 3:N:935:LYS:HZ3   | 1.67                     | 0.42              |
| 3:N:783:ARG:O    | 3:N:784:ASP:C     | 2.58                     | 0.42              |
| 3:N:965:GLU:OE2  | 3:N:969:ARG:NE    | 2.42                     | 0.42              |
| 5:P:287:THR:O    | 5:P:288:TYR:C     | 2.58                     | 0.42              |
| 5:P:312:GLN:OE1  | 5:P:312:GLN:CA    | 2.66                     | 0.42              |
| 1:A:91:ASN:HA    | 1:A:92:PRO:HD3    | 1.93                     | 0.42              |
| 1:A:96:THR:OG1   | 1:A:97:VAL:N      | 2.52                     | 0.42              |
| 1:B:10:VAL:O     | 1:B:10:VAL:HG23   | 2.20                     | 0.42              |
| 1:A:32:PHE:HZ    | 1:B:47:SER:HG     | 1.68                     | 0.42              |
| 2:C:1084:SER:OG  | 2:C:1085:PHE:N    | 2.53                     | 0.42              |
| 2:C:137:VAL:HG21 | 2:C:393:GLN:NE2   | 2.35                     | 0.42              |
| 2:C:369:PRO:HB2  | 2:C:370:ALA:H     | 1.66                     | 0.42              |
| 2:C:857:ASP:HB2  | 2:C:978:ARG:HG2   | 2.00                     | 0.42              |
| 3:D:493:ARG:O    | 3:D:1388:ARG:NH1  | 2.53                     | 0.42              |
| 3:D:1496:GLU:OE1 | 3:D:1499:ARG:HD2  | 2.20                     | 0.42              |
| 3:D:258:VAL:O    | 3:D:258:VAL:HG12  | 2.20                     | 0.42              |
| 3:D:34:TYR:CG    | 3:D:35:ARG:N      | 2.88                     | 0.42              |
| 3:D:209:ARG:HB2  | 3:D:389:GLU:HB3   | 2.00                     | 0.42              |
| 3:D:3:LYS:HB3    | 3:D:3:LYS:HE2     | 1.84                     | 0.42              |
| 3:D:530:VAL:HG22 | 3:D:534:ARG:C     | 2.40                     | 0.42              |
| 3:D:618:LEU:HD23 | 3:D:618:LEU:N     | 2.34                     | 0.42              |
| 5:F:160:ASP:O    | 5:F:164:LYS:HG3   | 2.20                     | 0.42              |
| 5:F:367:MET:HA   | 5:F:370:LYS:HE2   | 2.01                     | 0.42              |
| 5:F:383:LEU:HG   | 5:F:394:ARG:HD3   | 2.00                     | 0.42              |
| 1:K:221:HIS:C    | 1:K:223:THR:H     | 2.23                     | 0.42              |
| 1:L:117:VAL:HG12 | 1:L:118:ALA:N     | 2.35                     | 0.42              |
| 1:L:99:LEU:N     | 1:L:142:VAL:O     | 2.53                     | 0.42              |
| 1:L:22:GLU:HA    | 1:L:197:LEU:O     | 2.19                     | 0.42              |
| 2:M:1092:LEU:HG  | 2:M:1092:LEU:H    | 1.55                     | 0.42              |
| 2:M:397:GLU:OE2  | 2:M:631:SER:HA    | 2.19                     | 0.42              |
| 2:M:455:LEU:HD11 | 2:M:459:ALA:HB3   | 2.02                     | 0.42              |
| 2:M:480:THR:CG2  | 2:M:482:GLU:HB2   | 2.49                     | 0.42              |
| 3:N:127:LEU:O    | 3:N:130:SER:O     | 2.37                     | 0.42              |
| 3:N:1433:SER:HA  | 3:N:1457:ASP:CG   | 2.39                     | 0.42              |
| 3:N:1465:ASN:CG  | 3:N:1473:PRO:HD3  | 2.40                     | 0.42              |
| 3:N:1489:GLN:CG  | 3:N:1492:LEU:HD12 | 2.50                     | 0.42              |
| 3:N:217:LYS:HD2  | 3:N:262:LYS:HZ1   | 1.84                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:133:ILE:HG22 | 3:N:454:ALA:C    | 2.40                     | 0.42              |
| 3:N:880:ILE:O    | 3:N:881:LEU:C    | 2.58                     | 0.42              |
| 5:P:130:VAL:O    | 5:P:131:VAL:C    | 2.56                     | 0.42              |
| 1:A:104:GLU:CG   | 1:A:105:GLY:N    | 2.83                     | 0.42              |
| 1:A:110:LYS:O    | 1:A:129:ILE:HD12 | 2.20                     | 0.42              |
| 1:A:36:LEU:HD12  | 1:A:36:LEU:N     | 2.33                     | 0.42              |
| 1:B:36:LEU:O     | 1:B:37:GLY:C     | 2.58                     | 0.42              |
| 2:C:517:ARG:CA   | 2:C:520:GLU:HB2  | 2.50                     | 0.42              |
| 2:C:572:ILE:HA   | 2:C:640:ARG:HH22 | 1.84                     | 0.42              |
| 2:C:611:ILE:HD11 | 2:C:641:PRO:HB3  | 2.01                     | 0.42              |
| 2:C:705:ILE:HD12 | 2:C:705:ILE:H    | 1.85                     | 0.42              |
| 3:D:1258:ARG:NH2 | 3:D:1351:GLU:HG3 | 2.35                     | 0.42              |
| 3:D:1336:LEU:O   | 3:D:1340:GLY:CA  | 2.67                     | 0.42              |
| 3:D:1465:ASN:O   | 3:D:1468:LEU:HB3 | 2.20                     | 0.42              |
| 3:D:1479:ASP:N   | 3:D:1482:ARG:HG3 | 2.34                     | 0.42              |
| 3:D:1483:PHE:HD1 | 3:D:1483:PHE:H   | 1.65                     | 0.42              |
| 3:D:14:SER:O     | 3:D:17:LYS:N     | 2.53                     | 0.42              |
| 3:D:217:LYS:HB2  | 3:D:339:TRP:HE1  | 1.80                     | 0.42              |
| 3:D:266:GLU:O    | 3:D:314:PRO:HG3  | 2.19                     | 0.42              |
| 3:D:325:GLU:CD   | 3:D:332:TYR:HB3  | 2.40                     | 0.42              |
| 3:D:347:VAL:HG13 | 3:D:351:MET:CB   | 2.50                     | 0.42              |
| 3:D:539:ASP:HB3  | 3:D:600:LEU:HD13 | 2.02                     | 0.42              |
| 3:D:571:LYS:O    | 3:D:572:ARG:C    | 2.58                     | 0.42              |
| 3:D:764:LEU:HD23 | 3:D:767:HIS:NE2  | 2.35                     | 0.42              |
| 3:D:764:LEU:HG   | 3:D:766:ALA:H    | 1.85                     | 0.42              |
| 3:D:847:ASP:O    | 3:D:848:GLU:C    | 2.58                     | 0.42              |
| 4:E:22:VAL:O     | 4:E:23:VAL:C     | 2.58                     | 0.42              |
| 5:F:110:MET:CE   | 5:F:111:GLU:N    | 2.83                     | 0.42              |
| 5:F:123:ASP:HA   | 5:F:124:PRO:HD3  | 1.90                     | 0.42              |
| 5:F:161:GLN:O    | 5:F:165:SER:N    | 2.52                     | 0.42              |
| 5:F:262:VAL:O    | 5:F:265:VAL:N    | 2.53                     | 0.42              |
| 5:F:323:ASP:OD1  | 5:F:325:LYS:HD2  | 2.19                     | 0.42              |
| 5:F:398:ARG:CD   | 5:F:399:GLN:N    | 2.83                     | 0.42              |
| 1:K:179:PHE:HB3  | 1:K:197:LEU:CD2  | 2.50                     | 0.42              |
| 1:K:79:ILE:HG13  | 1:K:79:ILE:H     | 1.63                     | 0.42              |
| 2:M:252:LYS:C    | 2:M:255:ALA:HB3  | 2.39                     | 0.42              |
| 2:M:317:VAL:H    | 2:M:318:PRO:HD3  | 1.75                     | 0.42              |
| 2:M:373:VAL:CG1  | 2:M:374:ASN:N    | 2.77                     | 0.42              |
| 2:M:560:MET:O    | 2:M:564:MET:HB2  | 2.20                     | 0.42              |
| 2:M:610:ARG:HD2  | 2:M:622:GLU:HG2  | 2.01                     | 0.42              |
| 2:M:631:SER:O    | 2:M:634:GLY:N    | 2.43                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:86:LYS:NZ     | 2:M:811:PRO:O     | 2.53                     | 0.42              |
| 3:N:1047:LYS:HD2  | 3:N:1051:GLU:CG   | 2.49                     | 0.42              |
| 3:N:1223:ILE:HG22 | 3:N:1227:GLN:OE1  | 2.19                     | 0.42              |
| 3:N:1330:ILE:HG22 | 3:N:1331:ASP:N    | 2.33                     | 0.42              |
| 3:N:1376:MET:O    | 3:N:1377:LYS:C    | 2.58                     | 0.42              |
| 3:N:1465:ASN:ND2  | 3:N:1473:PRO:HD3  | 2.35                     | 0.42              |
| 3:N:244:GLU:CG    | 3:N:245:LEU:N     | 2.80                     | 0.42              |
| 3:N:272:LEU:CD1   | 3:N:282:TYR:HE1   | 2.32                     | 0.42              |
| 3:N:294:HIS:O     | 3:N:303:PRO:HA    | 2.20                     | 0.42              |
| 3:N:356:PRO:HD3   | 3:N:440:VAL:HB    | 2.01                     | 0.42              |
| 3:N:62:LYS:HE3    | 3:N:75:ARG:NH1    | 2.35                     | 0.42              |
| 2:M:874:LEU:HD12  | 3:N:784:ASP:OD1   | 2.20                     | 0.42              |
| 3:N:846:PRO:O     | 3:N:849:ALA:N     | 2.53                     | 0.42              |
| 3:N:857:ILE:C     | 3:N:858:VAL:HG23  | 2.39                     | 0.42              |
| 3:N:868:TYR:HB3   | 3:N:873:LEU:CD1   | 2.49                     | 0.42              |
| 3:N:868:TYR:HB3   | 3:N:873:LEU:HD11  | 2.01                     | 0.42              |
| 5:P:287:THR:O     | 5:P:291:ILE:HG22  | 2.19                     | 0.42              |
| 5:P:330:GLY:C     | 5:P:332:PHE:H     | 2.23                     | 0.42              |
| 1:A:216:GLU:O     | 1:A:219:ARG:HB3   | 2.20                     | 0.42              |
| 1:A:221:HIS:C     | 1:A:223:THR:H     | 2.24                     | 0.42              |
| 1:B:104:GLU:CA    | 1:B:132:LEU:HD13  | 2.43                     | 0.42              |
| 2:C:1040:LEU:HA   | 2:C:1040:LEU:HD23 | 1.91                     | 0.42              |
| 2:C:135:VAL:HG12  | 2:C:136:ILE:N     | 2.34                     | 0.42              |
| 2:C:267:TYR:HB2   | 2:C:272:ALA:H     | 1.83                     | 0.42              |
| 2:C:332:ARG:NH2   | 2:C:338:GLU:OE1   | 2.53                     | 0.42              |
| 2:C:504:GLU:HG3   | 2:C:507:ARG:HB2   | 2.02                     | 0.42              |
| 2:C:572:ILE:CG1   | 2:C:573:ARG:N     | 2.83                     | 0.42              |
| 2:C:58:ASP:C      | 2:C:60:GLY:H      | 2.23                     | 0.42              |
| 2:C:630:ARG:NE    | 2:C:634:GLY:HA2   | 2.35                     | 0.42              |
| 3:D:1035:ILE:O    | 3:D:1036:ARG:C    | 2.59                     | 0.42              |
| 3:D:102:ILE:HG23  | 3:D:103:TRP:N     | 2.34                     | 0.42              |
| 3:D:1150:ALA:HB3  | 3:D:1187:PRO:CB   | 2.49                     | 0.42              |
| 3:D:1259:VAL:O    | 3:D:1262:LEU:HB2  | 2.20                     | 0.42              |
| 3:D:1346:ARG:NH1  | 3:D:1346:ARG:CG   | 2.83                     | 0.42              |
| 3:D:432:TYR:H     | 3:D:432:TYR:HD1   | 1.67                     | 0.42              |
| 3:D:470:LEU:O     | 3:D:471:GLU:C     | 2.57                     | 0.42              |
| 3:D:64:LYS:HD3    | 5:F:377:ASP:OD2   | 2.20                     | 0.42              |
| 3:D:67:ARG:HD3    | 3:D:67:ARG:HA     | 1.80                     | 0.42              |
| 3:D:686:GLU:CD    | 3:D:686:GLU:H     | 2.23                     | 0.42              |
| 3:D:933:ALA:O     | 3:D:936:TYR:HB3   | 2.19                     | 0.42              |
| 5:F:117:SER:HA    | 5:F:127:ILE:HD11  | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:115:LYS:C    | 5:F:119:ILE:HG13 | 2.40                     | 0.42              |
| 5:F:119:ILE:O    | 5:F:119:ILE:HG22 | 2.20                     | 0.42              |
| 5:F:403:LYS:O    | 5:F:404:ALA:C    | 2.59                     | 0.42              |
| 1:K:109:VAL:HG13 | 1:K:113:ASP:OD2  | 2.20                     | 0.42              |
| 1:K:175:ARG:HH11 | 1:K:175:ARG:HG2  | 1.84                     | 0.42              |
| 1:K:56:VAL:CG1   | 1:K:57:TYR:N     | 2.83                     | 0.42              |
| 1:L:24:VAL:HG12  | 1:L:25:LEU:N     | 2.35                     | 0.42              |
| 1:L:66:SER:C     | 1:L:75:VAL:HG23  | 2.39                     | 0.42              |
| 2:M:1113:GLU:O   | 2:M:1113:GLU:CG  | 2.63                     | 0.42              |
| 2:M:141:HIS:CE1  | 2:M:332:ARG:HB3  | 2.55                     | 0.42              |
| 2:M:227:PHE:HD1  | 2:M:227:PHE:H    | 1.67                     | 0.42              |
| 2:M:258:TYR:O    | 2:M:290:LEU:CD1  | 2.67                     | 0.42              |
| 2:M:34:VAL:N     | 2:M:35:PRO:HD3   | 2.35                     | 0.42              |
| 2:M:354:GLY:HA2  | 2:M:357:GLU:OE2  | 2.19                     | 0.42              |
| 2:M:360:LEU:C    | 2:M:362:GLY:H    | 2.22                     | 0.42              |
| 2:M:414:GLY:N    | 2:M:419:THR:HG21 | 2.34                     | 0.42              |
| 2:M:431:HIS:HE1  | 2:M:432:ARG:HG2  | 1.82                     | 0.42              |
| 2:M:468:ARG:NE   | 2:M:487:THR:HG22 | 2.35                     | 0.42              |
| 2:M:540:PHE:HB3  | 2:M:544:THR:CG2  | 2.49                     | 0.42              |
| 2:M:857:ASP:HB3  | 2:M:978:ARG:HG2  | 2.01                     | 0.42              |
| 2:M:976:ASP:O    | 2:M:978:ARG:N    | 2.53                     | 0.42              |
| 3:N:1226:ALA:O   | 3:N:1229:ILE:N   | 2.53                     | 0.42              |
| 3:N:123:LEU:N    | 3:N:123:LEU:HD23 | 2.35                     | 0.42              |
| 3:N:1333:HIS:O   | 3:N:1334:GLN:C   | 2.58                     | 0.42              |
| 3:N:1347:TYR:O   | 3:N:1348:LEU:C   | 2.59                     | 0.42              |
| 3:N:134:VAL:O    | 3:N:134:VAL:HG12 | 2.19                     | 0.42              |
| 3:N:1429:LEU:HG  | 3:N:1429:LEU:O   | 2.20                     | 0.42              |
| 3:N:1464:GLU:O   | 3:N:1465:ASN:C   | 2.57                     | 0.42              |
| 3:N:371:ILE:HG13 | 3:N:372:ASP:N    | 2.30                     | 0.42              |
| 3:N:61:GLY:O     | 3:N:63:TYR:N     | 2.53                     | 0.42              |
| 3:N:730:PRO:O    | 3:N:732:VAL:N    | 2.53                     | 0.42              |
| 3:N:792:ILE:HG13 | 3:N:793:THR:N    | 2.31                     | 0.42              |
| 3:N:930:LEU:O    | 3:N:934:LEU:HD12 | 2.20                     | 0.42              |
| 3:N:944:THR:O    | 3:N:946:GLY:N    | 2.52                     | 0.42              |
| 3:N:956:ILE:HG12 | 3:N:1039:CYS:O   | 2.20                     | 0.42              |
| 4:O:80:VAL:HB    | 4:O:81:PRO:CD    | 2.49                     | 0.42              |
| 5:P:382:THR:HG23 | 5:P:397:ILE:CB   | 2.50                     | 0.42              |
| 5:P:409:LYS:O    | 5:P:412:GLU:N    | 2.53                     | 0.42              |
| 1:A:172:SER:HA   | 1:A:173:PRO:HD2  | 1.89                     | 0.41              |
| 1:A:43:ILE:O     | 1:A:47:SER:N     | 2.53                     | 0.41              |
| 1:B:214:ALA:O    | 1:B:215:VAL:C    | 2.58                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1047:HIS:NE2  | 3:D:754:PHE:CE1  | 2.88                     | 0.41              |
| 2:C:140:ILE:HD12  | 2:C:331:ARG:CZ   | 2.50                     | 0.41              |
| 2:C:182:VAL:CG1   | 2:C:193:LEU:HB3  | 2.50                     | 0.41              |
| 2:C:238:LEU:O     | 2:C:239:PHE:C    | 2.56                     | 0.41              |
| 2:C:270:GLY:O     | 2:C:272:ALA:N    | 2.53                     | 0.41              |
| 2:C:310:LEU:O     | 2:C:314:THR:HG23 | 2.20                     | 0.41              |
| 2:C:351:LEU:HD13  | 2:C:374:ASN:O    | 2.20                     | 0.41              |
| 2:C:461:VAL:CG2   | 2:C:467:ILE:HG12 | 2.50                     | 0.41              |
| 2:C:50:GLU:C      | 2:C:52:PHE:H     | 2.20                     | 0.41              |
| 2:C:52:PHE:HD1    | 2:C:54:ILE:H     | 1.67                     | 0.41              |
| 2:C:673:LEU:HB3   | 2:C:867:VAL:HB   | 2.01                     | 0.41              |
| 2:C:843:HIS:O     | 2:C:845:ASN:N    | 2.53                     | 0.41              |
| 2:C:894:GLY:CA    | 2:C:901:TYR:OH   | 2.68                     | 0.41              |
| 3:D:1076:GLY:O    | 3:D:1080:GLY:N   | 2.48                     | 0.41              |
| 3:D:1231:GLU:HB3  | 3:D:1232:PRO:CD  | 2.42                     | 0.41              |
| 3:D:1344:VAL:HG13 | 3:D:1345:GLU:H   | 1.79                     | 0.41              |
| 3:D:317:VAL:HB    | 3:D:339:TRP:HB3  | 2.01                     | 0.41              |
| 3:D:546:ARG:HH21  | 3:D:577:ALA:CB   | 2.33                     | 0.41              |
| 3:D:550:ARG:NH1   | 3:D:573:MET:CB   | 2.82                     | 0.41              |
| 3:D:591:VAL:O     | 3:D:593:ASN:N    | 2.53                     | 0.41              |
| 3:D:800:LYS:CE    | 3:D:826:PRO:CD   | 2.94                     | 0.41              |
| 3:D:884:ARG:O     | 3:D:885:ILE:C    | 2.58                     | 0.41              |
| 3:D:895:VAL:HA    | 3:D:898:GLU:CD   | 2.40                     | 0.41              |
| 5:F:291:ILE:CD1   | 5:F:295:MET:HB2  | 2.50                     | 0.41              |
| 1:K:182:GLU:O     | 1:K:194:LYS:HB3  | 2.20                     | 0.41              |
| 1:K:215:VAL:O     | 1:K:216:GLU:C    | 2.58                     | 0.41              |
| 1:L:138:LEU:HD12  | 1:L:139:ASN:H    | 1.85                     | 0.41              |
| 1:L:58:ILE:O      | 1:L:60:ASP:N     | 2.53                     | 0.41              |
| 1:L:81:ASN:O      | 1:L:84:GLU:HB2   | 2.20                     | 0.41              |
| 2:M:1049:LEU:O    | 2:M:1052:MET:HB3 | 2.20                     | 0.41              |
| 2:M:139:GLN:O     | 2:M:334:ARG:N    | 2.52                     | 0.41              |
| 2:M:193:LEU:O     | 2:M:194:VAL:C    | 2.58                     | 0.41              |
| 2:M:194:VAL:HA    | 2:M:197:LEU:HD12 | 1.98                     | 0.41              |
| 2:M:218:VAL:HG13  | 2:M:222:MET:CE   | 2.49                     | 0.41              |
| 2:M:38:LYS:CG     | 2:M:39:ARG:N     | 2.80                     | 0.41              |
| 2:M:402:SER:O     | 2:M:406:HIS:N    | 2.50                     | 0.41              |
| 2:M:503:LEU:HD12  | 2:M:508:ILE:CA   | 2.36                     | 0.41              |
| 2:M:504:GLU:HG3   | 2:M:504:GLU:O    | 2.20                     | 0.41              |
| 2:M:639:GLN:HG2   | 2:M:658:GLY:HA2  | 2.00                     | 0.41              |
| 3:N:1031:ASN:HB2  | 3:N:1032:PRO:HD2 | 2.02                     | 0.41              |
| 3:N:1082:ALA:O    | 3:N:1083:ASP:C   | 2.58                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1118:ILE:HG13 | 3:N:1188:VAL:HG13 | 2.02                     | 0.41              |
| 3:N:1397:LYS:C    | 3:N:1398:TRP:HD1  | 2.23                     | 0.41              |
| 3:N:15:PRO:O      | 3:N:19:ARG:HG3    | 2.19                     | 0.41              |
| 3:N:240:GLU:O     | 3:N:313:MET:N     | 2.40                     | 0.41              |
| 3:N:256:GLU:O     | 3:N:274:ARG:HB2   | 2.20                     | 0.41              |
| 3:N:262:LYS:NZ    | 3:N:339:TRP:HZ2   | 2.18                     | 0.41              |
| 3:N:259:VAL:HG11  | 3:N:293:VAL:CG1   | 2.50                     | 0.41              |
| 3:N:362:GLU:O     | 3:N:365:ASP:CB    | 2.67                     | 0.41              |
| 3:N:434:ARG:HH21  | 3:N:451:ASP:CG    | 2.23                     | 0.41              |
| 3:N:569:ASN:ND2   | 5:P:214:GLN:CD    | 2.73                     | 0.41              |
| 3:N:661:MET:O     | 3:N:662:GLU:C     | 2.59                     | 0.41              |
| 3:N:687:VAL:O     | 3:N:690:ALA:HB3   | 2.18                     | 0.41              |
| 3:N:983:LEU:HD22  | 3:N:987:GLU:CB    | 2.49                     | 0.41              |
| 4:O:33:HIS:CE1    | 4:O:89:MET:HG2    | 2.54                     | 0.41              |
| 5:P:128:ARG:HG3   | 5:P:128:ARG:HH11  | 1.85                     | 0.41              |
| 5:P:161:GLN:H     | 5:P:161:GLN:CD    | 2.23                     | 0.41              |
| 5:P:210:LEU:O     | 5:P:213:ILE:HB    | 2.19                     | 0.41              |
| 5:P:289:GLU:O     | 5:P:290:GLU:C     | 2.57                     | 0.41              |
| 2:C:1088:LEU:HA   | 2:C:1091:GLU:OE1  | 2.19                     | 0.41              |
| 2:C:1088:LEU:HD22 | 10:D:1529:NE6:H17 | 2.00                     | 0.41              |
| 2:C:1112:PHE:CD1  | 2:C:1116:ALA:HB2  | 2.55                     | 0.41              |
| 2:C:15:LEU:CD1    | 2:C:15:LEU:N      | 2.70                     | 0.41              |
| 2:C:270:GLY:O     | 2:C:271:GLU:C     | 2.59                     | 0.41              |
| 2:C:280:LYS:O     | 2:C:281:LEU:HD23  | 2.20                     | 0.41              |
| 2:C:285:LEU:HD11  | 2:C:289:THR:CA    | 2.50                     | 0.41              |
| 2:C:317:VAL:HG12  | 2:C:317:VAL:O     | 2.21                     | 0.41              |
| 2:C:462:ASP:HB2   | 2:C:463:GLU:OE1   | 2.20                     | 0.41              |
| 2:C:333:ILE:HG22  | 2:C:465:GLY:O     | 2.19                     | 0.41              |
| 2:C:676:ILE:O     | 2:C:677:MET:HB3   | 2.19                     | 0.41              |
| 3:D:1139:ASP:N    | 3:D:1139:ASP:OD1  | 2.51                     | 0.41              |
| 3:D:127:LEU:CD2   | 3:D:128:TYR:H     | 2.27                     | 0.41              |
| 3:D:1472:ILE:HG22 | 3:D:1474:ALA:O    | 2.19                     | 0.41              |
| 3:D:353:VAL:HG12  | 3:D:368:VAL:HG21  | 2.01                     | 0.41              |
| 3:D:466:LYS:O     | 3:D:468:LEU:N     | 2.54                     | 0.41              |
| 3:D:519:VAL:HG13  | 3:D:544:TYR:CZ    | 2.55                     | 0.41              |
| 3:D:563:PRO:C     | 3:D:565:ILE:H     | 2.23                     | 0.41              |
| 4:E:10:PHE:C      | 4:E:12:MET:N      | 2.73                     | 0.41              |
| 4:E:4:PRO:C       | 4:E:6:ILE:H       | 2.23                     | 0.41              |
| 4:E:50:THR:O      | 4:E:55:PHE:HE1    | 1.99                     | 0.41              |
| 4:E:66:LYS:O      | 4:E:69:LEU:HB2    | 2.20                     | 0.41              |
| 3:D:925:GLU:HG2   | 4:E:7:ASP:OD2     | 2.19                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:274:THR:HG22  | 5:F:278:LEU:HD21  | 2.02                     | 0.41              |
| 2:C:1068:GLU:OE1  | 5:F:345:ALA:HA    | 2.21                     | 0.41              |
| 5:F:380:GLU:C     | 5:F:382:THR:H     | 2.22                     | 0.41              |
| 1:K:36:LEU:HD12   | 1:K:36:LEU:N      | 2.35                     | 0.41              |
| 1:L:149:GLY:H     | 1:L:172:SER:HB2   | 1.85                     | 0.41              |
| 1:L:28:LEU:CD1    | 1:L:33:GLY:N      | 2.83                     | 0.41              |
| 2:M:1017:THR:HB   | 2:M:1019:GLN:HE21 | 1.84                     | 0.41              |
| 2:M:95:TYR:CD1    | 2:M:114:PHE:HB3   | 2.55                     | 0.41              |
| 2:M:118:ILE:HA    | 2:M:119:PRO:HD3   | 1.87                     | 0.41              |
| 2:M:217:LEU:C     | 2:M:219:GLN:N     | 2.70                     | 0.41              |
| 2:M:303:PHE:HD1   | 2:M:303:PHE:H     | 1.67                     | 0.41              |
| 2:M:676:ILE:O     | 2:M:677:MET:HB3   | 2.20                     | 0.41              |
| 2:M:914:ILE:O     | 2:M:915:LYS:C     | 2.58                     | 0.41              |
| 3:N:960:LYS:HE2   | 3:N:1063:GLU:OE1  | 2.19                     | 0.41              |
| 3:N:1262:LEU:HD22 | 3:N:1352:ILE:CG1  | 2.50                     | 0.41              |
| 3:N:156:GLU:OE2   | 3:N:156:GLU:N     | 2.47                     | 0.41              |
| 3:N:277:GLU:HG3   | 3:N:278:PRO:HD2   | 2.03                     | 0.41              |
| 3:N:225:LEU:N     | 3:N:331:VAL:O     | 2.53                     | 0.41              |
| 3:N:434:ARG:NH1   | 3:N:449:SER:OG    | 2.52                     | 0.41              |
| 3:N:481:MET:O     | 3:N:489:ARG:HG3   | 2.19                     | 0.41              |
| 3:N:84:ILE:C      | 3:N:86:ARG:H      | 2.23                     | 0.41              |
| 3:N:851:LEU:HD23  | 3:N:851:LEU:N     | 2.35                     | 0.41              |
| 3:N:855:HIS:O     | 3:N:856:GLY:C     | 2.59                     | 0.41              |
| 3:N:9:ARG:HG2     | 3:N:10:ILE:N      | 2.35                     | 0.41              |
| 5:P:245:GLN:CD    | 5:P:245:GLN:N     | 2.72                     | 0.41              |
| 1:B:6:LEU:C       | 1:B:8:ALA:N       | 2.74                     | 0.41              |
| 2:C:1095:LEU:O    | 3:D:101:HIS:NE2   | 2.54                     | 0.41              |
| 2:C:192:PRO:HB2   | 2:C:195:LEU:CD2   | 2.28                     | 0.41              |
| 2:C:266:ARG:HH11  | 2:C:266:ARG:CG    | 2.24                     | 0.41              |
| 2:C:311:PHE:N     | 2:C:311:PHE:CD2   | 2.88                     | 0.41              |
| 2:C:549:PHE:HE1   | 2:C:909:ALA:HB3   | 1.84                     | 0.41              |
| 2:C:572:ILE:HG13  | 2:C:573:ARG:H     | 1.84                     | 0.41              |
| 2:C:631:SER:O     | 2:C:632:ASN:C     | 2.59                     | 0.41              |
| 3:D:1031:ASN:CG   | 3:D:1034:GLN:HE21 | 2.24                     | 0.41              |
| 3:D:1041:LEU:HD12 | 3:D:1057:VAL:O    | 2.21                     | 0.41              |
| 3:D:1189:ARG:NH1  | 3:D:1203:LYS:HG3  | 2.36                     | 0.41              |
| 3:D:1333:HIS:O    | 3:D:1334:GLN:C    | 2.59                     | 0.41              |
| 3:D:1404:ASN:CA   | 3:D:1408:ILE:HB   | 2.46                     | 0.41              |
| 3:D:569:ASN:HD21  | 5:F:214:GLN:CD    | 2.23                     | 0.41              |
| 3:D:573:MET:H     | 3:D:573:MET:HG3   | 1.58                     | 0.41              |
| 3:D:710:ARG:O     | 3:D:712:GLY:N     | 2.52                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:630:VAL:N    | 3:D:744:GLN:HG2  | 2.34                     | 0.41              |
| 3:D:767:HIS:HA   | 3:D:924:MET:CE   | 2.50                     | 0.41              |
| 3:D:794:GLN:O    | 3:D:861:GLN:HA   | 2.20                     | 0.41              |
| 3:D:71:LYS:N     | 3:D:80:VAL:CG2   | 2.83                     | 0.41              |
| 3:D:821:VAL:C    | 3:D:823:LEU:N    | 2.73                     | 0.41              |
| 3:D:901:GLN:O    | 3:D:904:VAL:HG22 | 2.20                     | 0.41              |
| 2:C:681:GLY:HA3  | 3:D:939:PHE:CE1  | 2.55                     | 0.41              |
| 4:E:26:ARG:HE    | 4:E:30:LEU:HD22  | 1.85                     | 0.41              |
| 5:F:170:HIS:O    | 5:F:173:TYR:N    | 2.53                     | 0.41              |
| 5:F:205:ARG:HD2  | 5:F:251:ILE:HD13 | 2.01                     | 0.41              |
| 5:F:287:THR:H    | 5:F:290:GLU:CD   | 2.24                     | 0.41              |
| 1:K:73:GLU:CG    | 1:K:130:ALA:HA   | 2.50                     | 0.41              |
| 1:K:5:LYS:C      | 1:K:7:LYS:N      | 2.72                     | 0.41              |
| 2:M:1014:SER:HB3 | 2:M:1019:GLN:H   | 1.85                     | 0.41              |
| 2:M:1066:ALA:O   | 2:M:1067:TYR:C   | 2.57                     | 0.41              |
| 2:M:252:LYS:CA   | 2:M:255:ALA:HB3  | 2.51                     | 0.41              |
| 2:M:461:VAL:CG2  | 2:M:467:ILE:HG12 | 2.51                     | 0.41              |
| 2:M:432:ARG:NH1  | 2:M:518:LYS:O    | 2.52                     | 0.41              |
| 2:M:679:PHE:HA   | 3:N:943:THR:CG2  | 2.37                     | 0.41              |
| 2:M:37:GLU:CB    | 2:M:71:TYR:HE2   | 2.34                     | 0.41              |
| 3:N:794:GLN:HG3  | 3:N:1017:PHE:CZ  | 2.55                     | 0.41              |
| 3:N:1070:TYR:O   | 3:N:1071:PHE:C   | 2.57                     | 0.41              |
| 3:N:1379:VAL:O   | 3:N:1392:GLY:HA2 | 2.19                     | 0.41              |
| 3:N:1436:SER:O   | 3:N:1439:SER:N   | 2.52                     | 0.41              |
| 3:N:265:GLU:HB2  | 3:N:316:GLN:OE1  | 2.20                     | 0.41              |
| 3:N:32:ILE:CG2   | 3:N:37:LEU:HA    | 2.50                     | 0.41              |
| 3:N:131:LYS:HA   | 3:N:456:MET:CE   | 2.51                     | 0.41              |
| 3:N:692:GLU:O    | 3:N:695:ILE:HB   | 2.21                     | 0.41              |
| 3:N:711:LEU:CD2  | 3:N:778:LEU:HD23 | 2.43                     | 0.41              |
| 2:M:1098:ASP:O   | 3:N:9:ARG:O      | 2.38                     | 0.41              |
| 5:P:151:LEU:O    | 5:P:156:VAL:HG22 | 2.20                     | 0.41              |
| 5:P:184:ARG:O    | 5:P:185:GLN:C    | 2.58                     | 0.41              |
| 5:P:251:ILE:O    | 5:P:255:ALA:HB2  | 2.21                     | 0.41              |
| 5:P:393:THR:CG2  | 5:P:394:ARG:N    | 2.83                     | 0.41              |
| 5:P:406:ARG:O    | 5:P:407:LYS:C    | 2.59                     | 0.41              |
| 1:B:58:ILE:O     | 1:B:59:GLU:C     | 2.58                     | 0.41              |
| 2:C:267:TYR:HD2  | 2:C:268:ASP:H    | 1.68                     | 0.41              |
| 2:C:437:ARG:NH2  | 2:C:487:THR:C    | 2.74                     | 0.41              |
| 2:C:41:ASN:O     | 2:C:46:ALA:N     | 2.53                     | 0.41              |
| 2:C:486:MET:HE1  | 2:C:491:GLU:HA   | 2.01                     | 0.41              |
| 2:C:694:LEU:CD2  | 2:C:697:ARG:HH22 | 2.34                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:726:ILE:O     | 2:C:728:HIS:N    | 2.54                     | 0.41              |
| 2:C:897:LEU:HD21  | 2:C:921:ALA:N    | 2.35                     | 0.41              |
| 3:D:1197:ARG:O    | 3:D:1198:TYR:CD1 | 2.74                     | 0.41              |
| 3:D:1106:VAL:HG11 | 3:D:1474:ALA:CB  | 2.50                     | 0.41              |
| 3:D:1217:ILE:HD13 | 3:D:1480:PHE:CE2 | 2.55                     | 0.41              |
| 3:D:192:ALA:H     | 3:D:195:VAL:HB   | 1.84                     | 0.41              |
| 3:D:403:PHE:CD1   | 3:D:404:GLU:N    | 2.88                     | 0.41              |
| 3:D:403:PHE:CE2   | 3:D:442:ASN:HB3  | 2.54                     | 0.41              |
| 3:D:472:ALA:O     | 3:D:473:LEU:C    | 2.57                     | 0.41              |
| 3:D:95:LEU:CB     | 3:D:515:GLU:HA   | 2.41                     | 0.41              |
| 3:D:612:GLY:O     | 3:D:616:GLN:HG2  | 2.20                     | 0.41              |
| 3:D:660:LYS:O     | 3:D:661:MET:C    | 2.58                     | 0.41              |
| 3:D:822:ALA:HB3   | 3:D:824:ASN:ND2  | 2.35                     | 0.41              |
| 5:F:220:LEU:O     | 5:F:224:VAL:HG23 | 2.20                     | 0.41              |
| 5:F:260:ILE:HD11  | 5:F:264:MET:HB3  | 2.01                     | 0.41              |
| 5:F:271:LEU:HB2   | 5:F:272:SER:H    | 1.71                     | 0.41              |
| 5:F:367:MET:HG2   | 5:F:370:LYS:HE2  | 2.01                     | 0.41              |
| 1:K:206:THR:HG22  | 1:K:208:LEU:N    | 2.35                     | 0.41              |
| 1:L:55:SER:CB     | 1:L:166:PRO:HA   | 2.51                     | 0.41              |
| 2:M:148:PHE:H     | 2:M:323:ASP:CG   | 2.20                     | 0.41              |
| 2:M:45:GLN:HA     | 2:M:48:PHE:HD1   | 1.85                     | 0.41              |
| 2:M:588:VAL:HG23  | 2:M:596:TYR:OH   | 2.19                     | 0.41              |
| 2:M:713:ARG:HA    | 2:M:818:GLY:O    | 2.19                     | 0.41              |
| 2:M:987:ILE:HG22  | 2:M:988:VAL:O    | 2.21                     | 0.41              |
| 3:N:1021:TYR:O    | 3:N:1022:VAL:C   | 2.59                     | 0.41              |
| 3:N:1078:ARG:O    | 3:N:1079:LYS:C   | 2.58                     | 0.41              |
| 3:N:1117:TYR:HD1  | 3:N:1118:ILE:N   | 2.17                     | 0.41              |
| 3:N:1226:ALA:O    | 3:N:1227:GLN:C   | 2.57                     | 0.41              |
| 3:N:139:GLY:CA    | 3:N:147:VAL:HB   | 2.49                     | 0.41              |
| 3:N:1489:GLN:NE2  | 4:O:72:ARG:C     | 2.74                     | 0.41              |
| 3:N:15:PRO:HD2    | 3:N:16:GLU:OE2   | 2.20                     | 0.41              |
| 3:N:191:LEU:HB3   | 3:N:195:VAL:HB   | 2.03                     | 0.41              |
| 3:N:217:LYS:HE3   | 3:N:341:GLU:OE1  | 2.19                     | 0.41              |
| 3:N:436:GLU:HB2   | 3:N:445:ARG:O    | 2.20                     | 0.41              |
| 3:N:531:ASP:O     | 3:N:532:GLY:C    | 2.59                     | 0.41              |
| 3:N:547:LEU:O     | 3:N:548:ILE:C    | 2.59                     | 0.41              |
| 3:N:572:ARG:HD3   | 5:P:83:GLN:OE1   | 2.20                     | 0.41              |
| 3:N:69:GLU:HG3    | 3:N:70:GLY:N     | 2.36                     | 0.41              |
| 3:N:827:ILE:CG2   | 3:N:837:GLY:HA3  | 2.50                     | 0.41              |
| 3:N:1489:GLN:HE22 | 4:O:73:LEU:N     | 2.16                     | 0.41              |
| 4:O:81:PRO:O      | 4:O:85:LEU:HD21  | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:P:373:LYS:C    | 5:P:375:LEU:N    | 2.74                     | 0.41              |
| 5:P:382:THR:O    | 5:P:385:GLU:N    | 2.54                     | 0.41              |
| 1:A:222:LEU:O    | 1:A:225:PHE:HD1  | 2.02                     | 0.41              |
| 1:A:33:GLY:HA2   | 1:A:195:LEU:HB2  | 2.03                     | 0.41              |
| 1:B:112:ARG:HG3  | 1:B:113:ASP:N    | 2.35                     | 0.41              |
| 2:C:1001:VAL:O   | 2:C:1004:LYS:HB3 | 2.20                     | 0.41              |
| 2:C:1041:GLU:O   | 2:C:1044:GLY:N   | 2.54                     | 0.41              |
| 2:C:1078:GLU:HA  | 2:C:1079:PRO:HD3 | 1.77                     | 0.41              |
| 2:C:333:ILE:HG21 | 2:C:461:VAL:HG21 | 2.02                     | 0.41              |
| 2:C:375:SER:O    | 2:C:376:ARG:C    | 2.59                     | 0.41              |
| 2:C:583:LEU:O    | 2:C:584:GLU:C    | 2.59                     | 0.41              |
| 2:C:662:GLU:C    | 2:C:664:GLY:N    | 2.74                     | 0.41              |
| 2:C:754:ILE:HG12 | 2:C:791:ARG:HD2  | 2.02                     | 0.41              |
| 3:D:1074:SER:O   | 3:D:1077:ALA:N   | 2.53                     | 0.41              |
| 3:D:1315:ASP:O   | 3:D:1316:GLY:C   | 2.59                     | 0.41              |
| 3:D:1374:GLN:OE1 | 3:D:1374:GLN:HA  | 2.20                     | 0.41              |
| 3:D:1466:VAL:C   | 3:D:1468:LEU:H   | 2.22                     | 0.41              |
| 3:D:219:GLU:O    | 3:D:337:LEU:HG   | 2.21                     | 0.41              |
| 3:D:262:LYS:O    | 3:D:268:ALA:HA   | 2.20                     | 0.41              |
| 3:D:241:ILE:CG1  | 3:D:312:ARG:CZ   | 2.97                     | 0.41              |
| 3:D:361:VAL:HG13 | 3:D:379:ALA:CB   | 2.32                     | 0.41              |
| 3:D:443:VAL:CG1  | 3:D:444:VAL:N    | 2.84                     | 0.41              |
| 3:D:735:ALA:C    | 3:D:737:ASN:H    | 2.23                     | 0.41              |
| 3:D:932:ASP:HA   | 3:D:935:LYS:HB3  | 2.03                     | 0.41              |
| 3:D:986:ARG:O    | 3:D:987:GLU:C    | 2.59                     | 0.41              |
| 3:D:1494:ALA:HB2 | 4:E:92:ILE:HD11  | 2.01                     | 0.41              |
| 5:F:135:ILE:C    | 5:F:137:GLY:H    | 2.23                     | 0.41              |
| 5:F:209:PHE:HA   | 5:F:212:LEU:HG   | 2.02                     | 0.41              |
| 1:K:110:LYS:O    | 1:K:113:ASP:OD2  | 2.39                     | 0.41              |
| 1:K:222:LEU:HA   | 1:K:225:PHE:CD1  | 2.54                     | 0.41              |
| 1:K:9:PRO:HA     | 1:K:27:PRO:HD2   | 2.02                     | 0.41              |
| 1:K:89:PHE:CD2   | 1:K:94:LEU:HB3   | 2.55                     | 0.41              |
| 1:L:165:ILE:HG23 | 1:L:166:PRO:HD2  | 2.01                     | 0.41              |
| 1:L:28:LEU:CD2   | 1:L:29:GLU:N     | 2.82                     | 0.41              |
| 2:M:150:PRO:HA   | 2:M:158:TYR:CB   | 2.20                     | 0.41              |
| 2:M:185:LYS:NZ   | 2:M:190:LYS:HZ2  | 2.17                     | 0.41              |
| 2:M:202:TYR:CB   | 2:M:207:LEU:HD21 | 2.51                     | 0.41              |
| 2:M:180:GLY:HA2  | 2:M:223:ASP:OD2  | 2.21                     | 0.41              |
| 2:M:141:HIS:CB   | 2:M:418:LEU:HD22 | 2.50                     | 0.41              |
| 2:M:691:SER:HB3  | 2:M:868:ASP:HA   | 2.02                     | 0.41              |
| 2:M:780:GLU:OE1  | 2:M:780:GLU:HA   | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:795:GLY:O    | 2:M:796:GLU:HG2   | 2.21                     | 0.41              |
| 2:M:83:CYS:SG    | 2:M:90:TYR:HA     | 2.61                     | 0.41              |
| 2:M:922:PHE:CE2  | 2:M:964:LYS:HB2   | 2.56                     | 0.41              |
| 3:N:1147:ARG:HB3 | 3:N:1188:VAL:HG23 | 2.01                     | 0.41              |
| 3:N:1346:ARG:O   | 3:N:1347:TYR:C    | 2.58                     | 0.41              |
| 3:N:1399:ASP:HB3 | 3:N:1400:VAL:H    | 1.76                     | 0.41              |
| 3:N:272:LEU:HD12 | 3:N:282:TYR:HE1   | 1.86                     | 0.41              |
| 3:N:250:LEU:CD1  | 3:N:306:GLU:HG2   | 2.51                     | 0.41              |
| 3:N:309:GLY:O    | 3:N:311:LEU:HG    | 2.20                     | 0.41              |
| 3:N:217:LYS:HD2  | 3:N:339:TRP:CZ2   | 2.56                     | 0.41              |
| 3:N:39:PRO:HB3   | 3:N:45:PHE:C      | 2.41                     | 0.41              |
| 3:N:521:PRO:HD2  | 3:N:524:LEU:HD12  | 2.02                     | 0.41              |
| 3:N:631:ILE:CG2  | 3:N:745:MET:HB2   | 2.49                     | 0.41              |
| 2:M:1045:ALA:HA  | 3:N:758:GLU:HB3   | 2.02                     | 0.41              |
| 5:P:117:SER:OG   | 5:P:124:PRO:HG3   | 2.20                     | 0.41              |
| 3:N:560:GLN:HA   | 5:P:132:ARG:HH12  | 1.85                     | 0.41              |
| 1:A:123:MET:O    | 1:A:125:PRO:HD2   | 2.21                     | 0.41              |
| 2:C:196:LEU:O    | 2:C:200:LEU:HG    | 2.21                     | 0.41              |
| 2:C:343:GLN:HG2  | 2:C:385:PHE:CB    | 2.50                     | 0.41              |
| 2:C:396:ASP:CB   | 2:C:406:HIS:HD2   | 2.34                     | 0.41              |
| 2:C:449:ILE:O    | 2:C:451:LEU:HG    | 2.20                     | 0.41              |
| 2:C:444:PRO:CG   | 2:C:452:ILE:HB    | 2.51                     | 0.41              |
| 2:C:459:ALA:HB1  | 2:C:467:ILE:CG2   | 2.50                     | 0.41              |
| 2:C:677:MET:N    | 2:C:871:LEU:O     | 2.53                     | 0.41              |
| 2:C:876:VAL:O    | 2:C:877:PRO:C     | 2.59                     | 0.41              |
| 3:D:1304:LYS:O   | 3:D:1305:LEU:HB3  | 2.21                     | 0.41              |
| 3:D:1447:LEU:O   | 3:D:1450:ALA:N    | 2.54                     | 0.41              |
| 3:D:342:PRO:O    | 3:D:343:LYS:CG    | 2.67                     | 0.41              |
| 3:D:470:LEU:HG   | 3:D:470:LEU:H     | 1.62                     | 0.41              |
| 3:D:546:ARG:HG3  | 3:D:547:LEU:H     | 1.85                     | 0.41              |
| 3:D:547:LEU:O    | 3:D:548:ILE:C     | 2.58                     | 0.41              |
| 4:E:7:ASP:CA     | 4:E:10:PHE:HD1    | 2.28                     | 0.41              |
| 4:E:26:ARG:NE    | 4:E:30:LEU:HD22   | 2.34                     | 0.41              |
| 4:E:26:ARG:NH2   | 4:E:38:THR:HA     | 2.34                     | 0.41              |
| 5:F:135:ILE:CD1  | 5:F:181:GLU:HB3   | 2.50                     | 0.41              |
| 5:F:170:HIS:HA   | 5:F:173:TYR:CD1   | 2.56                     | 0.41              |
| 5:F:231:ARG:HB2  | 5:F:233:PHE:CE2   | 2.55                     | 0.41              |
| 5:F:346:THR:O    | 5:F:349:LEU:HB3   | 2.21                     | 0.41              |
| 1:K:143:ARG:NH1  | 1:K:158:ILE:HD12  | 2.35                     | 0.41              |
| 1:K:36:LEU:O     | 1:K:37:GLY:C      | 2.58                     | 0.41              |
| 1:K:86:VAL:HG13  | 1:K:123:MET:CB    | 2.43                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:L:109:VAL:HG12 | 1:L:129:ILE:HD12  | 2.01                     | 0.41              |
| 1:L:176:ARG:HD3  | 3:N:884:ARG:HH22  | 1.83                     | 0.41              |
| 2:M:135:VAL:HG23 | 2:M:395:LYS:HA    | 2.02                     | 0.41              |
| 2:M:194:VAL:C    | 2:M:197:LEU:HG    | 2.41                     | 0.41              |
| 2:M:293:PHE:CD1  | 2:M:293:PHE:C     | 2.94                     | 0.41              |
| 2:M:27:ARG:C     | 2:M:29:ALA:H      | 2.23                     | 0.41              |
| 2:M:360:LEU:HB2  | 2:M:361:MET:SD    | 2.61                     | 0.41              |
| 2:M:461:VAL:HG23 | 2:M:467:ILE:HG12  | 2.02                     | 0.41              |
| 2:M:770:GLU:OE1  | 3:N:65:ARG:NH2    | 2.53                     | 0.41              |
| 2:M:854:PRO:O    | 2:M:857:ASP:OD2   | 2.38                     | 0.41              |
| 2:M:874:LEU:O    | 2:M:876:VAL:N     | 2.54                     | 0.41              |
| 3:N:133:ILE:HG13 | 3:N:153:LEU:HD23  | 2.02                     | 0.41              |
| 3:N:1424:VAL:O   | 3:N:1425:THR:C    | 2.58                     | 0.41              |
| 3:N:1442:ASN:C   | 3:N:1442:ASN:ND2  | 2.74                     | 0.41              |
| 3:N:179:VAL:HG13 | 3:N:180:LYS:N     | 2.36                     | 0.41              |
| 3:N:213:VAL:CG1  | 3:N:215:TYR:CE2   | 3.04                     | 0.41              |
| 3:N:22:SER:C     | 3:N:24:GLY:N      | 2.74                     | 0.41              |
| 3:N:230:TRP:CE2  | 3:N:233:LYS:HE3   | 2.55                     | 0.41              |
| 3:N:217:LYS:CB   | 3:N:339:TRP:HE1   | 2.15                     | 0.41              |
| 3:N:348:GLN:H    | 3:N:351:MET:CE    | 2.15                     | 0.41              |
| 3:N:472:ALA:O    | 3:N:473:LEU:C     | 2.58                     | 0.41              |
| 3:N:637:LEU:O    | 3:N:935:LYS:NZ    | 2.53                     | 0.41              |
| 4:O:42:PRO:O     | 4:O:43:GLU:C      | 2.59                     | 0.41              |
| 3:N:573:MET:HE1  | 5:P:211:ASP:OD1   | 2.21                     | 0.41              |
| 5:P:224:VAL:O    | 5:P:227:PHE:HB3   | 2.20                     | 0.41              |
| 5:P:300:ASP:OD1  | 5:P:301:ALA:N     | 2.54                     | 0.41              |
| 1:A:179:PHE:HB3  | 1:A:197:LEU:CD2   | 2.50                     | 0.41              |
| 1:A:38:ASN:N     | 1:A:179:PHE:CE2   | 2.88                     | 0.41              |
| 1:B:112:ARG:C    | 1:B:114:PHE:N     | 2.71                     | 0.41              |
| 1:B:206:THR:HG22 | 1:B:208:LEU:N     | 2.36                     | 0.41              |
| 2:C:424:GLY:O    | 2:C:425:PHE:C     | 2.58                     | 0.41              |
| 2:C:512:ARG:HD2  | 2:C:523:ILE:HG12  | 2.02                     | 0.41              |
| 3:D:1006:ALA:O   | 3:D:1009:LYS:HB3  | 2.21                     | 0.41              |
| 3:D:1114:THR:HA  | 3:D:1195:GLN:CD   | 2.41                     | 0.41              |
| 3:D:1114:THR:HA  | 3:D:1195:GLN:NE2  | 2.35                     | 0.41              |
| 3:D:121:THR:O    | 3:D:125:GLN:HB3   | 2.21                     | 0.41              |
| 3:D:1299:PHE:N   | 3:D:1299:PHE:CD1  | 2.86                     | 0.41              |
| 3:D:1307:LYS:N   | 3:D:1307:LYS:CE   | 2.76                     | 0.41              |
| 3:D:1400:VAL:HA  | 3:D:1408:ILE:HD12 | 2.02                     | 0.41              |
| 3:D:1418:LYS:HA  | 3:D:1419:PRO:HD3  | 1.95                     | 0.41              |
| 3:D:1491:THR:O   | 3:D:1491:THR:HG22 | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:156:GLU:HG2   | 3:D:157:GLU:N    | 2.35                     | 0.41              |
| 3:D:214:GLU:HG2   | 3:D:342:PRO:CA   | 2.50                     | 0.41              |
| 3:D:353:VAL:HG23  | 3:D:353:VAL:O    | 2.21                     | 0.41              |
| 3:D:205:TYR:OH    | 3:D:445:ARG:NH2  | 2.53                     | 0.41              |
| 3:D:162:ARG:O     | 3:D:449:SER:HB2  | 2.20                     | 0.41              |
| 3:D:508:ARG:HB2   | 3:D:511:TRP:CE2  | 2.56                     | 0.41              |
| 3:D:536:ALA:C     | 5:F:317:LEU:HD21 | 2.41                     | 0.41              |
| 3:D:550:ARG:NH1   | 3:D:573:MET:C    | 2.74                     | 0.41              |
| 3:D:72:VAL:CG1    | 3:D:73:CYS:N     | 2.83                     | 0.41              |
| 3:D:965:GLU:C     | 3:D:967:ALA:N    | 2.73                     | 0.41              |
| 5:F:116:LEU:O     | 5:F:119:ILE:N    | 2.53                     | 0.41              |
| 5:F:278:LEU:O     | 5:F:279:GLN:C    | 2.57                     | 0.41              |
| 5:F:417:LYS:O     | 5:F:419:ARG:N    | 2.53                     | 0.41              |
| 1:K:213:GLN:O     | 1:K:216:GLU:HB3  | 2.20                     | 0.41              |
| 1:L:188:GLN:HG3   | 1:L:189:ARG:N    | 2.35                     | 0.41              |
| 1:L:56:VAL:CG1    | 1:L:57:TYR:N     | 2.83                     | 0.41              |
| 2:M:1015:LEU:HD12 | 5:P:335:ASP:HB2  | 2.02                     | 0.41              |
| 2:M:63:GLY:H      | 2:M:103:LYS:HB2  | 1.85                     | 0.41              |
| 2:M:1050:GLN:O    | 2:M:1051:GLU:C   | 2.59                     | 0.41              |
| 2:M:186:VAL:HG22  | 2:M:187:ASN:N    | 2.35                     | 0.41              |
| 2:M:437:ARG:HG3   | 2:M:437:ARG:NH1  | 2.36                     | 0.41              |
| 2:M:754:ILE:HG12  | 2:M:791:ARG:CD   | 2.50                     | 0.41              |
| 3:N:101:HIS:C     | 3:N:101:HIS:ND1  | 2.73                     | 0.41              |
| 3:N:1031:ASN:O    | 3:N:1034:GLN:HB2 | 2.21                     | 0.41              |
| 3:N:1066:THR:HB   | 3:N:1069:GLU:HG3 | 2.03                     | 0.41              |
| 3:N:1118:ILE:CG1  | 3:N:1190:SER:HB2 | 2.49                     | 0.41              |
| 3:N:1224:VAL:HA   | 3:N:1227:GLN:OE1 | 2.21                     | 0.41              |
| 3:N:133:ILE:O     | 3:N:153:LEU:HB3  | 2.21                     | 0.41              |
| 3:N:1388:ARG:HG2  | 3:N:1391:GLU:HG3 | 2.02                     | 0.41              |
| 3:N:14:SER:O      | 3:N:18:ILE:HG13  | 2.21                     | 0.41              |
| 3:N:322:VAL:HG22  | 3:N:323:GLU:N    | 2.36                     | 0.41              |
| 3:N:350:HIS:O     | 3:N:370:ALA:HA   | 2.21                     | 0.41              |
| 3:N:210:ARG:HD2   | 3:N:389:GLU:OE2  | 2.21                     | 0.41              |
| 3:N:536:ALA:HB1   | 5:P:317:LEU:HD23 | 2.01                     | 0.41              |
| 3:N:564:GLU:HA    | 3:N:567:ILE:HB   | 2.03                     | 0.41              |
| 3:N:650:LEU:O     | 3:N:651:GLU:C    | 2.57                     | 0.41              |
| 3:N:664:LYS:HB2   | 3:N:666:ILE:HG12 | 2.01                     | 0.41              |
| 3:N:792:ILE:O     | 3:N:878:GLY:HA3  | 2.20                     | 0.41              |
| 4:O:76:GLY:HA3    | 4:O:79:LEU:CD2   | 2.42                     | 0.41              |
| 5:P:308:LEU:N     | 5:P:308:LEU:HD23 | 2.33                     | 0.41              |
| 5:P:353:GLU:CA    | 5:P:356:LYS:HB2  | 2.51                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:P:364:ARG:O    | 5:P:367:MET:HG3  | 2.21                     | 0.41              |
| 5:P:97:GLU:HG3   | 5:P:97:GLU:H     | 1.71                     | 0.41              |
| 1:A:151:VAL:O    | 1:A:156:HIS:HE1  | 2.04                     | 0.41              |
| 1:B:20:TYR:C     | 1:B:207:PRO:HG2  | 2.41                     | 0.41              |
| 1:B:20:TYR:CG    | 1:B:21:GLY:N     | 2.88                     | 0.41              |
| 2:C:62:GLY:HA3   | 2:C:103:LYS:CG   | 2.50                     | 0.41              |
| 2:C:1086:ARG:O   | 2:C:1087:VAL:C   | 2.59                     | 0.41              |
| 2:C:1118:LYS:O   | 2:C:1119:ARG:HB2 | 2.20                     | 0.41              |
| 2:C:167:LYS:O    | 2:C:167:LYS:HG2  | 2.20                     | 0.41              |
| 2:C:334:ARG:HD2  | 2:C:418:LEU:HD13 | 2.02                     | 0.41              |
| 2:C:382:ILE:O    | 2:C:383:ARG:C    | 2.58                     | 0.41              |
| 2:C:446:GLY:O    | 2:C:449:ILE:N    | 2.45                     | 0.41              |
| 2:C:573:ARG:HB2  | 2:C:670:GLN:HE22 | 1.83                     | 0.41              |
| 2:C:60:GLY:C     | 2:C:62:GLY:H     | 2.24                     | 0.41              |
| 2:C:611:ILE:HG22 | 2:C:612:VAL:N    | 2.36                     | 0.41              |
| 2:C:680:ASP:H    | 3:D:943:THR:HG1  | 1.63                     | 0.41              |
| 2:C:724:ARG:CD   | 2:C:738:ASP:HA   | 2.50                     | 0.41              |
| 3:D:1019:PRO:O   | 3:D:1022:VAL:HB  | 2.21                     | 0.41              |
| 3:D:119:SER:H    | 3:D:123:LEU:HG   | 1.80                     | 0.41              |
| 3:D:1269:LYS:N   | 3:D:1269:LYS:CD  | 2.84                     | 0.41              |
| 3:D:1347:TYR:O   | 3:D:1348:LEU:C   | 2.58                     | 0.41              |
| 3:D:1384:PRO:CB  | 3:D:1387:SER:O   | 2.68                     | 0.41              |
| 3:D:247:GLU:HA   | 3:D:248:PRO:HA   | 1.94                     | 0.41              |
| 3:D:318:ARG:CG   | 3:D:319:ALA:H    | 2.33                     | 0.41              |
| 3:D:221:ALA:O    | 3:D:334:THR:HG22 | 2.20                     | 0.41              |
| 3:D:403:PHE:CD1  | 3:D:403:PHE:C    | 2.93                     | 0.41              |
| 3:D:46:ASP:C     | 3:D:48:ARG:H     | 2.24                     | 0.41              |
| 3:D:46:ASP:OD2   | 3:D:48:ARG:HB2   | 2.21                     | 0.41              |
| 3:D:536:ALA:HA   | 5:F:315:VAL:O    | 2.21                     | 0.41              |
| 3:D:541:ASN:O    | 3:D:545:ARG:CG   | 2.69                     | 0.41              |
| 3:D:592:THR:HG23 | 3:D:600:LEU:HD21 | 2.02                     | 0.41              |
| 3:D:700:VAL:O    | 3:D:701:LEU:HD23 | 2.21                     | 0.41              |
| 3:D:630:VAL:HA   | 3:D:744:GLN:HG2  | 2.01                     | 0.41              |
| 5:F:367:MET:HB3  | 5:F:371:LEU:CG   | 2.50                     | 0.41              |
| 5:F:372:ARG:HG3  | 5:F:378:GLY:C    | 2.39                     | 0.41              |
| 5:F:382:THR:C    | 5:F:384:GLU:N    | 2.74                     | 0.41              |
| 5:F:385:GLU:CA   | 5:F:388:ALA:HB3  | 2.30                     | 0.41              |
| 1:L:111:ALA:HB2  | 1:L:127:LEU:HB3  | 2.02                     | 0.41              |
| 1:L:143:ARG:C    | 1:L:143:ARG:CD   | 2.88                     | 0.41              |
| 2:M:198:ARG:HG3  | 2:M:231:PRO:HA   | 2.03                     | 0.41              |
| 2:M:255:ALA:O    | 2:M:257:VAL:N    | 2.53                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:408:ARG:CD    | 2:M:542:VAL:HG13 | 2.51                     | 0.41              |
| 2:M:928:LYS:HG2   | 2:M:932:GLU:HG3  | 2.03                     | 0.41              |
| 3:N:1078:ARG:C    | 3:N:1080:GLY:N   | 2.74                     | 0.41              |
| 3:N:1129:THR:CG2  | 3:N:1130:ARG:N   | 2.84                     | 0.41              |
| 3:N:1174:LEU:HG   | 3:N:1174:LEU:H   | 1.55                     | 0.41              |
| 3:N:187:LYS:HG3   | 3:N:198:ARG:HG3  | 2.03                     | 0.41              |
| 3:N:204:LEU:HD12  | 3:N:205:TYR:N    | 2.35                     | 0.41              |
| 3:N:325:GLU:H     | 3:N:331:VAL:HG13 | 1.86                     | 0.41              |
| 3:N:581:LEU:O     | 3:N:582:LEU:C    | 2.59                     | 0.41              |
| 3:N:583:ASP:HA    | 3:N:602:SER:OG   | 2.20                     | 0.41              |
| 3:N:806:PHE:CE1   | 3:N:816:HIS:CE1  | 3.09                     | 0.41              |
| 3:N:812:ALA:HA    | 3:N:816:HIS:N    | 2.35                     | 0.41              |
| 4:O:6:ILE:HD11    | 4:O:10:PHE:CZ    | 2.56                     | 0.41              |
| 5:P:102:LEU:HD21  | 5:P:187:LEU:H    | 1.86                     | 0.41              |
| 5:P:239:ALA:C     | 5:P:241:TRP:N    | 2.72                     | 0.41              |
| 5:P:268:ILE:CA    | 5:P:271:LEU:HG   | 2.51                     | 0.41              |
| 5:P:403:LYS:HZ3   | 5:P:407:LYS:HE2  | 1.86                     | 0.41              |
| 1:A:87:VAL:HG21   | 1:A:144:VAL:HG11 | 2.03                     | 0.41              |
| 1:A:77:GLU:O      | 1:A:81:ASN:ND2   | 2.54                     | 0.41              |
| 1:B:95:GLN:NE2    | 1:B:146:ARG:NH1  | 2.69                     | 0.41              |
| 2:C:1016:ILE:O    | 2:C:1018:GLN:HG2 | 2.21                     | 0.41              |
| 2:C:101:ILE:HG12  | 2:C:107:LEU:HA   | 2.01                     | 0.41              |
| 2:C:172:ILE:HG23  | 2:C:184:MET:HE3  | 2.02                     | 0.41              |
| 2:C:316:GLY:C     | 2:C:318:PRO:HD3  | 2.40                     | 0.41              |
| 2:C:468:ARG:HG2   | 2:C:487:THR:HG22 | 2.03                     | 0.41              |
| 2:C:589:ARG:HG2   | 2:C:596:TYR:CE2  | 2.56                     | 0.41              |
| 2:C:631:SER:HB3   | 2:C:635:THR:H    | 1.82                     | 0.41              |
| 2:C:773:LEU:O     | 2:C:774:LEU:C    | 2.59                     | 0.41              |
| 2:C:854:PRO:O     | 2:C:855:VAL:C    | 2.58                     | 0.41              |
| 3:D:1253:THR:CG2  | 3:D:1257:PRO:HB2 | 2.50                     | 0.41              |
| 3:D:1278:ASP:HB3  | 3:D:1318:TYR:OH  | 2.21                     | 0.41              |
| 3:D:1296:SER:C    | 3:D:1298:GLY:N   | 2.74                     | 0.41              |
| 3:D:1258:ARG:HH21 | 3:D:1351:GLU:CG  | 2.33                     | 0.41              |
| 3:D:1464:GLU:HG3  | 3:D:1465:ASN:H   | 1.85                     | 0.41              |
| 3:D:1495:ILE:HA   | 4:E:84:ARG:HD3   | 2.03                     | 0.41              |
| 3:D:1096:ARG:HG2  | 6:D:1528:PO4:O2  | 2.21                     | 0.41              |
| 3:D:499:VAL:O     | 3:D:500:ARG:C    | 2.60                     | 0.41              |
| 3:D:552:ASN:HA    | 3:D:555:LYS:CD   | 2.38                     | 0.41              |
| 3:D:564:GLU:CA    | 3:D:567:ILE:HB   | 2.50                     | 0.41              |
| 3:D:939:PHE:O     | 3:D:940:THR:C    | 2.58                     | 0.41              |
| 3:D:989:TYR:O     | 3:D:990:ASP:C    | 2.58                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:85:LEU:CD2    | 4:E:85:LEU:H      | 2.27                     | 0.41              |
| 3:D:567:ILE:HG13  | 5:F:140:ARG:NH2   | 2.36                     | 0.41              |
| 5:F:151:LEU:C     | 5:F:153:PRO:HD2   | 2.41                     | 0.41              |
| 5:F:152:ASP:O     | 5:F:156:VAL:HG21  | 2.21                     | 0.41              |
| 5:F:161:GLN:O     | 5:F:165:SER:CB    | 2.68                     | 0.41              |
| 5:F:245:GLN:O     | 5:F:246:ALA:C     | 2.59                     | 0.41              |
| 5:F:370:LYS:O     | 5:F:374:GLY:N     | 2.53                     | 0.41              |
| 1:K:73:GLU:HB3    | 1:K:78:ILE:HG12   | 2.03                     | 0.41              |
| 2:M:138:SER:O     | 2:M:410:ILE:HG23  | 2.20                     | 0.41              |
| 2:M:396:ASP:HA    | 2:M:633:GLN:HE22  | 1.86                     | 0.41              |
| 2:M:66:LEU:HA     | 2:M:66:LEU:HD12   | 1.82                     | 0.41              |
| 2:M:69:LEU:O      | 2:M:70:GLU:HG3    | 2.21                     | 0.41              |
| 2:M:577:PRO:HG3   | 2:M:993:PHE:CG    | 2.56                     | 0.41              |
| 3:N:1311:LEU:HD12 | 3:N:1312:LEU:N    | 2.32                     | 0.41              |
| 3:N:1400:VAL:O    | 3:N:1404:ASN:ND2  | 2.54                     | 0.41              |
| 3:N:1380:GLU:N    | 3:N:1420:LEU:HD22 | 2.35                     | 0.41              |
| 3:N:497:GLU:O     | 3:N:498:VAL:C     | 2.59                     | 0.41              |
| 3:N:690:ALA:O     | 3:N:694:VAL:HG23  | 2.21                     | 0.41              |
| 3:N:1476:THR:CB   | 4:O:21:VAL:HG23   | 2.44                     | 0.41              |
| 4:O:46:PRO:HG2    | 4:O:63:TRP:CG     | 2.55                     | 0.41              |
| 5:P:261:PRO:HB2   | 5:P:264:MET:HB2   | 2.03                     | 0.41              |
| 5:P:267:THR:O     | 5:P:268:ILE:C     | 2.59                     | 0.41              |
| 1:A:43:ILE:HG23   | 1:A:47:SER:CB     | 2.51                     | 0.41              |
| 1:B:19:GLU:HG2    | 1:B:203:GLY:HA2   | 2.02                     | 0.41              |
| 1:B:58:ILE:HA     | 1:B:140:MET:HA    | 2.03                     | 0.41              |
| 2:C:139:GLN:HG2   | 2:C:391:LEU:CD2   | 2.51                     | 0.41              |
| 2:C:300:ASP:OD1   | 2:C:303:PHE:N     | 2.53                     | 0.41              |
| 2:C:410:ILE:N     | 2:C:453:THR:O     | 2.50                     | 0.41              |
| 2:C:575:GLN:C     | 2:C:667:ALA:HB1   | 2.40                     | 0.41              |
| 2:C:841:ASN:C     | 2:C:843:HIS:N     | 2.74                     | 0.41              |
| 3:D:1046:GLN:HB2  | 3:D:1052:THR:HA   | 2.01                     | 0.41              |
| 3:D:1149:LEU:HD23 | 3:D:1160:LEU:O    | 2.21                     | 0.41              |
| 3:D:1194:CYS:HB2  | 3:D:1204:CYS:HB3  | 2.03                     | 0.41              |
| 3:D:142:LEU:HD22  | 3:D:144:GLY:O     | 2.20                     | 0.41              |
| 3:D:217:LYS:HB2   | 3:D:339:TRP:CD1   | 2.56                     | 0.41              |
| 3:D:264:LEU:HB2   | 3:D:267:GLY:CA    | 2.50                     | 0.41              |
| 3:D:550:ARG:HD2   | 3:D:577:ALA:HB2   | 2.02                     | 0.41              |
| 3:D:564:GLU:HA    | 3:D:567:ILE:CB    | 2.51                     | 0.41              |
| 3:D:922:LEU:O     | 3:D:923:GLY:O     | 2.38                     | 0.41              |
| 5:F:222:ARG:CG    | 5:F:242:TRP:CZ3   | 3.04                     | 0.41              |
| 5:F:257:THR:O     | 5:F:258:ILE:HD13  | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:269:ASN:C     | 5:F:271:LEU:N     | 2.74                     | 0.41              |
| 1:L:28:LEU:HD23   | 1:L:29:GLU:H      | 1.84                     | 0.41              |
| 2:M:218:VAL:HG13  | 2:M:222:MET:HE2   | 2.03                     | 0.41              |
| 2:M:370:ALA:C     | 2:M:372:LEU:N     | 2.75                     | 0.41              |
| 2:M:398:THR:HA    | 2:M:633:GLN:CG    | 2.44                     | 0.41              |
| 2:M:457:ALA:HB2   | 2:M:545:ASN:ND2   | 2.36                     | 0.41              |
| 2:M:558:ALA:O     | 2:M:561:GLY:N     | 2.53                     | 0.41              |
| 2:M:674:VAL:HG22  | 2:M:675:ALA:N     | 2.36                     | 0.41              |
| 2:M:711:GLU:OE1   | 2:M:711:GLU:N     | 2.54                     | 0.41              |
| 2:M:890:LEU:O     | 2:M:893:ALA:N     | 2.54                     | 0.41              |
| 2:M:985:GLY:HA2   | 2:M:986:PRO:HD3   | 1.72                     | 0.41              |
| 3:N:1001:GLU:O    | 3:N:1002:LYS:C    | 2.58                     | 0.41              |
| 3:N:1333:HIS:C    | 3:N:1337:GLU:OE2  | 2.59                     | 0.41              |
| 3:N:1229:ILE:HA   | 3:N:1363:LEU:HD11 | 2.03                     | 0.41              |
| 3:N:1379:VAL:HG22 | 3:N:1393:GLN:O    | 2.21                     | 0.41              |
| 3:N:261:LEU:HD23  | 3:N:270:LEU:CA    | 2.51                     | 0.41              |
| 3:N:378:ILE:HG12  | 3:N:379:ALA:N     | 2.35                     | 0.41              |
| 3:N:128:TYR:CZ    | 3:N:461:ILE:HG13  | 2.55                     | 0.41              |
| 3:N:464:LEU:HD23  | 3:N:464:LEU:N     | 2.36                     | 0.41              |
| 3:N:583:ASP:OD1   | 3:N:604:THR:HB    | 2.21                     | 0.41              |
| 3:N:606:ILE:O     | 3:N:607:LEU:C     | 2.59                     | 0.41              |
| 3:N:62:LYS:HE3    | 3:N:75:ARG:HD3    | 2.02                     | 0.41              |
| 3:N:794:GLN:HA    | 3:N:794:GLN:OE1   | 2.21                     | 0.41              |
| 3:N:92:HIS:C      | 3:N:93:ILE:HG13   | 2.41                     | 0.41              |
| 3:N:963:TYR:O     | 3:N:967:ALA:CB    | 2.69                     | 0.41              |
| 5:P:194:LEU:HD13  | 5:P:194:LEU:C     | 2.41                     | 0.41              |
| 5:P:409:LYS:CG    | 5:P:410:TYR:H     | 2.33                     | 0.41              |
| 1:A:179:PHE:C     | 1:A:179:PHE:CD1   | 2.94                     | 0.41              |
| 1:A:48:ILE:HA     | 1:A:49:PRO:HD3    | 1.72                     | 0.41              |
| 1:B:176:ARG:C     | 1:B:200:TRP:HD1   | 2.24                     | 0.41              |
| 1:B:48:ILE:HA     | 1:B:49:PRO:HD2    | 1.81                     | 0.41              |
| 1:B:58:ILE:O      | 1:B:58:ILE:HG23   | 2.21                     | 0.41              |
| 2:C:1072:LYS:HG2  | 2:C:1072:LYS:H    | 1.65                     | 0.41              |
| 2:C:1088:LEU:O    | 2:C:1089:VAL:C    | 2.58                     | 0.41              |
| 2:C:151:ASP:H     | 2:C:158:TYR:HB3   | 1.86                     | 0.41              |
| 2:C:227:PHE:O     | 2:C:233:GLU:OE1   | 2.38                     | 0.41              |
| 2:C:30:LEU:HA     | 2:C:44:ILE:HD12   | 2.03                     | 0.41              |
| 2:C:503:LEU:CD1   | 2:C:508:ILE:HA    | 2.37                     | 0.41              |
| 2:C:517:ARG:O     | 2:C:518:LYS:C     | 2.59                     | 0.41              |
| 2:C:673:LEU:HB3   | 2:C:867:VAL:HA    | 2.02                     | 0.41              |
| 2:C:683:ASN:HD22  | 2:C:683:ASN:C     | 2.24                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:790:LEU:HD12 | 2:C:791:ARG:H     | 1.83                     | 0.41              |
| 2:C:807:ARG:CB   | 2:C:807:ARG:CZ    | 2.99                     | 0.41              |
| 2:C:958:THR:O    | 2:C:962:GLN:HG3   | 2.20                     | 0.41              |
| 2:C:839:LEU:HA   | 2:C:995:MET:O     | 2.21                     | 0.41              |
| 2:C:435:TYR:HD1  | 3:D:1071:PHE:CD2  | 2.39                     | 0.41              |
| 3:D:1147:ARG:HB2 | 3:D:1166:LEU:CD1  | 2.48                     | 0.41              |
| 3:D:1190:SER:OG  | 3:D:1191:PRO:HD2  | 2.20                     | 0.41              |
| 3:D:1117:TYR:CA  | 3:D:1193:THR:HG21 | 2.51                     | 0.41              |
| 3:D:126:VAL:HG12 | 3:D:127:LEU:N     | 2.36                     | 0.41              |
| 3:D:1345:GLU:OE2 | 3:D:1376:MET:HG3  | 2.20                     | 0.41              |
| 3:D:1405:GLU:CG  | 3:D:1406:ARG:N    | 2.83                     | 0.41              |
| 3:D:245:LEU:HG   | 3:D:309:GLY:CA    | 2.50                     | 0.41              |
| 3:D:273:ARG:O    | 3:D:274:ARG:C     | 2.59                     | 0.41              |
| 3:D:297:ILE:CG2  | 3:D:298:VAL:N     | 2.83                     | 0.41              |
| 3:D:528:VAL:CG1  | 3:D:529:GLN:N     | 2.84                     | 0.41              |
| 3:D:539:ASP:CB   | 3:D:600:LEU:HB3   | 2.50                     | 0.41              |
| 3:D:612:GLY:O    | 3:D:615:ARG:HG2   | 2.21                     | 0.41              |
| 3:D:662:GLU:C    | 3:D:664:LYS:H     | 2.23                     | 0.41              |
| 3:D:740:PHE:CD1  | 3:D:740:PHE:N     | 2.89                     | 0.41              |
| 3:D:896:ALA:O    | 3:D:900:ILE:HG13  | 2.20                     | 0.41              |
| 3:D:950:GLY:C    | 3:D:952:ASP:N     | 2.74                     | 0.41              |
| 5:F:102:LEU:HD21 | 5:F:187:LEU:H     | 1.85                     | 0.41              |
| 5:F:208:SER:O    | 5:F:209:PHE:C     | 2.59                     | 0.41              |
| 5:F:291:ILE:O    | 5:F:294:ALA:N     | 2.54                     | 0.41              |
| 5:F:408:LEU:O    | 5:F:411:HIS:HB3   | 2.20                     | 0.41              |
| 1:L:58:ILE:CG1   | 1:L:140:MET:HB3   | 2.45                     | 0.41              |
| 2:M:640:ARG:HD2  | 2:M:642:ARG:NH2   | 2.36                     | 0.41              |
| 2:M:944:LEU:O    | 2:M:947:ALA:HB3   | 2.21                     | 0.41              |
| 3:N:102:ILE:C    | 3:N:104:PHE:N     | 2.75                     | 0.41              |
| 3:N:1103:HIS:N   | 3:N:1104:GLU:OE1  | 2.54                     | 0.41              |
| 3:N:124:GLU:O    | 3:N:128:TYR:HD2   | 2.04                     | 0.41              |
| 3:N:298:VAL:CB   | 3:N:300:LYS:HE3   | 2.49                     | 0.41              |
| 3:N:325:GLU:CD   | 3:N:332:TYR:HB3   | 2.41                     | 0.41              |
| 3:N:493:ARG:O    | 3:N:496:LEU:HB3   | 2.20                     | 0.41              |
| 3:N:640:HIS:ND1  | 3:N:641:GLN:HG3   | 2.36                     | 0.41              |
| 3:N:73:CYS:HB3   | 3:N:76:CYS:SG     | 2.61                     | 0.41              |
| 3:N:879:ARG:O    | 3:N:882:PHE:HB3   | 2.20                     | 0.41              |
| 4:O:29:GLN:HB3   | 4:O:29:GLN:HE21   | 1.69                     | 0.41              |
| 5:P:146:GLY:HA3  | 5:P:149:GLU:CD    | 2.42                     | 0.41              |
| 5:P:156:VAL:HG22 | 5:P:156:VAL:H     | 1.67                     | 0.41              |
| 5:P:202:TYR:CD1  | 5:P:202:TYR:N     | 2.89                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:280:GLN:CG    | 5:P:281:GLU:N     | 2.80                     | 0.41              |
| 5:P:356:LYS:HB3   | 5:P:417:LYS:HZ3   | 1.85                     | 0.41              |
| 5:P:381:HIS:O     | 5:P:384:GLU:HG3   | 2.20                     | 0.41              |
| 1:A:31:GLY:N      | 1:A:193:ASP:OD2   | 2.54                     | 0.40              |
| 1:A:179:PHE:HB3   | 1:A:197:LEU:HD21  | 2.03                     | 0.40              |
| 1:A:40:LEU:HA     | 1:A:43:ILE:HD12   | 2.03                     | 0.40              |
| 1:A:5:LYS:HZ2     | 1:A:29:GLU:N      | 2.18                     | 0.40              |
| 2:C:1076:VAL:HA   | 2:C:1077:PRO:HD3  | 1.85                     | 0.40              |
| 2:C:1093:GLN:O    | 2:C:1096:ALA:N    | 2.52                     | 0.40              |
| 2:C:96:ALA:O      | 2:C:113:VAL:HG22  | 2.21                     | 0.40              |
| 2:C:165:LEU:HA    | 2:C:165:LEU:HD23  | 1.78                     | 0.40              |
| 2:C:455:LEU:HD11  | 2:C:459:ALA:HB3   | 2.03                     | 0.40              |
| 2:C:631:SER:CB    | 2:C:635:THR:OG1   | 2.69                     | 0.40              |
| 2:C:666:LEU:CD1   | 2:C:668:LEU:HG    | 2.42                     | 0.40              |
| 2:C:707:ARG:HG2   | 2:C:708:TYR:N     | 2.35                     | 0.40              |
| 2:C:726:ILE:CD1   | 2:C:728:HIS:HB2   | 2.51                     | 0.40              |
| 2:C:961:GLU:O     | 2:C:962:GLN:C     | 2.58                     | 0.40              |
| 2:C:915:LYS:O     | 2:C:968:LEU:HD22  | 2.20                     | 0.40              |
| 3:D:1023:MET:O    | 3:D:1024:ALA:C    | 2.59                     | 0.40              |
| 3:D:1190:SER:OG   | 3:D:1191:PRO:CD   | 2.69                     | 0.40              |
| 3:D:1107:VAL:HG12 | 3:D:1217:ILE:HG23 | 2.03                     | 0.40              |
| 3:D:123:LEU:O     | 3:D:124:GLU:C     | 2.59                     | 0.40              |
| 3:D:1281:VAL:HG21 | 3:D:1313:VAL:CG2  | 2.51                     | 0.40              |
| 3:D:1274:ILE:HD11 | 3:D:1334:GLN:HB3  | 2.02                     | 0.40              |
| 3:D:1415:VAL:O    | 3:D:1415:VAL:HG23 | 2.21                     | 0.40              |
| 3:D:1438:ALA:HA   | 3:D:1446:VAL:HG21 | 2.03                     | 0.40              |
| 3:D:1439:SER:OG   | 3:D:1463:LYS:NZ   | 2.53                     | 0.40              |
| 3:D:152:LEU:CD1   | 3:D:153:LEU:H     | 2.33                     | 0.40              |
| 3:D:159:ARG:C     | 3:D:161:LEU:N     | 2.74                     | 0.40              |
| 3:D:268:ALA:CB    | 3:D:290:PRO:HG3   | 2.51                     | 0.40              |
| 3:D:608:SER:HB2   | 3:D:614:PHE:CE1   | 2.56                     | 0.40              |
| 3:D:661:MET:O     | 3:D:664:LYS:O     | 2.40                     | 0.40              |
| 2:C:685:GLU:HG3   | 3:D:739:ASP:HB3   | 2.03                     | 0.40              |
| 3:D:826:PRO:HB3   | 3:D:828:LYS:HZ1   | 1.86                     | 0.40              |
| 3:D:851:LEU:H     | 3:D:851:LEU:CD2   | 2.32                     | 0.40              |
| 3:D:875:THR:HG22  | 3:D:876:SER:N     | 2.25                     | 0.40              |
| 3:D:882:PHE:O     | 3:D:885:ILE:HB    | 2.21                     | 0.40              |
| 5:F:172:ARG:O     | 5:F:176:ILE:HG13  | 2.21                     | 0.40              |
| 5:F:193:ARG:O     | 5:F:194:LEU:C     | 2.59                     | 0.40              |
| 1:K:206:THR:CB    | 1:K:209:GLU:HG3   | 2.36                     | 0.40              |
| 1:K:42:ARG:O      | 1:K:43:ILE:C      | 2.59                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:99:LEU:HA    | 1:L:99:LEU:HD23  | 1.90                     | 0.40              |
| 2:M:631:SER:O    | 2:M:632:ASN:C    | 2.60                     | 0.40              |
| 2:M:807:ARG:HA   | 2:M:821:GLU:CB   | 2.50                     | 0.40              |
| 2:M:869:VAL:HG22 | 2:M:870:ILE:N    | 2.35                     | 0.40              |
| 2:M:874:LEU:C    | 2:M:876:VAL:H    | 2.25                     | 0.40              |
| 1:K:183:ASP:CG   | 2:M:938:LYS:HE3  | 2.42                     | 0.40              |
| 2:M:73:LEU:HB3   | 2:M:93:PRO:O     | 2.21                     | 0.40              |
| 2:M:567:GLN:CB   | 2:M:997:LEU:HD22 | 2.51                     | 0.40              |
| 3:N:106:LYS:NZ   | 3:N:106:LYS:HB3  | 2.36                     | 0.40              |
| 3:N:1445:HIS:O   | 3:N:1448:THR:HB  | 2.20                     | 0.40              |
| 3:N:149:LYS:CE   | 3:N:151:GLN:HG3  | 2.47                     | 0.40              |
| 3:N:186:VAL:CG1  | 3:N:187:LYS:N    | 2.83                     | 0.40              |
| 3:N:32:ILE:HD12  | 3:N:527:MET:HG2  | 2.03                     | 0.40              |
| 3:N:496:LEU:O    | 3:N:497:GLU:C    | 2.59                     | 0.40              |
| 3:N:574:LEU:O    | 3:N:578:VAL:HG23 | 2.21                     | 0.40              |
| 3:N:661:MET:HA   | 3:N:666:ILE:HD11 | 2.02                     | 0.40              |
| 3:N:686:GLU:O    | 3:N:687:VAL:C    | 2.59                     | 0.40              |
| 3:N:832:ARG:HG3  | 3:N:832:ARG:O    | 2.20                     | 0.40              |
| 3:N:860:LEU:HA   | 3:N:877:PRO:CB   | 2.46                     | 0.40              |
| 3:N:957:PRO:HG2  | 3:N:1007:VAL:CA  | 2.48                     | 0.40              |
| 3:N:996:TRP:HA   | 3:N:999:THR:OG1  | 2.19                     | 0.40              |
| 5:P:154:LYS:O    | 5:P:155:THR:C    | 2.59                     | 0.40              |
| 5:P:215:GLU:O    | 5:P:218:GLN:HG3  | 2.20                     | 0.40              |
| 5:P:343:ASP:O    | 5:P:344:ALA:C    | 2.60                     | 0.40              |
| 3:N:391:ALA:HB2  | 5:P:97:GLU:OE2   | 2.20                     | 0.40              |
| 1:A:209:GLU:CA   | 1:A:212:ASN:HD22 | 2.34                     | 0.40              |
| 1:B:106:PRO:CA   | 1:B:133:GLU:HA   | 2.40                     | 0.40              |
| 1:B:221:HIS:C    | 1:B:223:THR:H    | 2.24                     | 0.40              |
| 1:B:48:ILE:HG22  | 1:B:173:PRO:CD   | 2.51                     | 0.40              |
| 2:C:1064:ASN:ND2 | 2:C:1064:ASN:H   | 2.19                     | 0.40              |
| 2:C:1066:ALA:O   | 2:C:1067:TYR:C   | 2.60                     | 0.40              |
| 2:C:267:TYR:HB2  | 2:C:272:ALA:N    | 2.36                     | 0.40              |
| 2:C:328:LEU:HD12 | 2:C:437:ARG:HD2  | 2.03                     | 0.40              |
| 2:C:41:ASN:O     | 2:C:46:ALA:CB    | 2.69                     | 0.40              |
| 2:C:514:VAL:O    | 2:C:514:VAL:HG23 | 2.20                     | 0.40              |
| 2:C:640:ARG:O    | 2:C:657:ASP:N    | 2.50                     | 0.40              |
| 2:C:668:LEU:HD23 | 2:C:668:LEU:HA   | 1.93                     | 0.40              |
| 2:C:728:HIS:CD2  | 2:C:730:SER:O    | 2.74                     | 0.40              |
| 2:C:806:LEU:HB2  | 2:C:822:VAL:HG22 | 2.03                     | 0.40              |
| 2:C:813:VAL:HG11 | 2:C:815:LEU:HG   | 2.01                     | 0.40              |
| 2:C:944:LEU:O    | 2:C:945:ARG:C    | 2.60                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:998:TYR:HE2   | 2:C:1000:MET:HA  | 1.86                     | 0.40              |
| 3:D:1041:LEU:HG   | 3:D:1043:GLY:CA  | 2.51                     | 0.40              |
| 3:D:1199:GLY:O    | 3:D:1373:ARG:NH1 | 2.54                     | 0.40              |
| 3:D:142:LEU:C     | 3:D:142:LEU:HD12 | 2.41                     | 0.40              |
| 3:D:244:GLU:OE2   | 3:D:310:LEU:CD2  | 2.69                     | 0.40              |
| 3:D:341:GLU:HA    | 3:D:342:PRO:HD2  | 1.87                     | 0.40              |
| 3:D:387:LEU:H     | 3:D:387:LEU:CD1  | 2.16                     | 0.40              |
| 3:D:481:MET:O     | 3:D:489:ARG:CD   | 2.69                     | 0.40              |
| 3:D:504:ASP:O     | 3:D:506:GLY:N    | 2.54                     | 0.40              |
| 3:D:731:LEU:O     | 3:D:734:GLU:HG2  | 2.22                     | 0.40              |
| 3:D:73:CYS:O      | 3:D:77:GLY:HA2   | 2.21                     | 0.40              |
| 3:D:936:TYR:CE2   | 3:D:940:THR:HG21 | 2.57                     | 0.40              |
| 5:F:247:ILE:O     | 5:F:248:ASN:C    | 2.58                     | 0.40              |
| 2:M:1036:GLU:CD   | 2:M:1036:GLU:N   | 2.74                     | 0.40              |
| 2:M:1102:LEU:O    | 3:N:5:VAL:CA     | 2.67                     | 0.40              |
| 2:M:157:ARG:HG3   | 2:M:158:TYR:N    | 2.37                     | 0.40              |
| 2:M:233:GLU:HB2   | 2:M:237:ARG:NH2  | 2.37                     | 0.40              |
| 2:M:461:VAL:HA    | 2:M:466:PHE:O    | 2.20                     | 0.40              |
| 2:M:469:THR:HA    | 2:M:470:PRO:HD3  | 1.96                     | 0.40              |
| 2:M:504:GLU:HG3   | 2:M:507:ARG:HD3  | 2.02                     | 0.40              |
| 2:M:603:VAL:HG21  | 2:M:644:VAL:O    | 2.21                     | 0.40              |
| 2:M:738:ASP:OD1   | 2:M:738:ASP:N    | 2.54                     | 0.40              |
| 2:M:879:ARG:HH11  | 2:M:879:ARG:HG2  | 1.86                     | 0.40              |
| 2:M:921:ALA:O     | 2:M:922:PHE:C    | 2.60                     | 0.40              |
| 2:M:937:ASP:O     | 2:M:940:GLU:N    | 2.54                     | 0.40              |
| 3:N:1068:LEU:HD12 | 3:N:1068:LEU:HA  | 1.78                     | 0.40              |
| 3:N:110:SER:O     | 3:N:111:LYS:C    | 2.58                     | 0.40              |
| 3:N:112:ILE:HG23  | 3:N:512:MET:CE   | 2.51                     | 0.40              |
| 3:N:1123:PHE:CA   | 3:N:1133:ARG:O   | 2.69                     | 0.40              |
| 3:N:1165:TYR:CZ   | 3:N:1214:PRO:HB3 | 2.56                     | 0.40              |
| 3:N:141:ILE:HB    | 3:N:450:TYR:HB3  | 2.04                     | 0.40              |
| 3:N:1436:SER:O    | 3:N:1437:ALA:C   | 2.59                     | 0.40              |
| 3:N:246:PRO:HD2   | 3:N:307:ALA:O    | 2.21                     | 0.40              |
| 3:N:223:LEU:O     | 3:N:332:TYR:CD1  | 2.74                     | 0.40              |
| 3:N:792:ILE:HD13  | 3:N:941:PHE:HE1  | 1.84                     | 0.40              |
| 3:N:854:ALA:C     | 3:N:856:GLY:N    | 2.74                     | 0.40              |
| 3:N:934:LEU:O     | 3:N:935:LYS:C    | 2.60                     | 0.40              |
| 3:N:950:GLY:O     | 3:N:953:ASP:HB2  | 2.22                     | 0.40              |
| 3:N:972:LEU:O     | 3:N:973:GLN:C    | 2.60                     | 0.40              |
| 5:P:235:PHE:O     | 5:P:238:TYR:N    | 2.54                     | 0.40              |
| 1:A:175:ARG:O     | 1:A:176:ARG:HB2  | 2.20                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1004:LYS:HG2  | 2:C:1005:MET:N   | 2.36                     | 0.40              |
| 2:C:1019:GLN:O    | 2:C:1020:PRO:C   | 2.60                     | 0.40              |
| 2:C:172:ILE:H     | 2:C:172:ILE:HG13 | 1.70                     | 0.40              |
| 2:C:328:LEU:HD12  | 2:C:433:THR:C    | 2.42                     | 0.40              |
| 1:A:70:GLY:H      | 2:C:607:ASP:CG   | 2.25                     | 0.40              |
| 2:C:906:PHE:HZ    | 3:D:1070:TYR:CD2 | 2.39                     | 0.40              |
| 2:C:90:TYR:O      | 2:C:119:PRO:HA   | 2.21                     | 0.40              |
| 2:C:974:LEU:O     | 2:C:983:ILE:HG13 | 2.20                     | 0.40              |
| 3:D:1149:LEU:HB3  | 3:D:1163:GLY:H   | 1.86                     | 0.40              |
| 3:D:1179:GLU:C    | 3:D:1181:GLY:N   | 2.75                     | 0.40              |
| 3:D:1339:LYS:CB   | 3:D:1343:ALA:CB  | 2.99                     | 0.40              |
| 3:D:1403:LEU:HB3  | 3:D:1408:ILE:CD1 | 2.51                     | 0.40              |
| 3:D:1440:PHE:CD2  | 3:D:1440:PHE:N   | 2.86                     | 0.40              |
| 3:D:1447:LEU:O    | 3:D:1449:GLU:N   | 2.54                     | 0.40              |
| 3:D:226:PRO:HB2   | 3:D:231:VAL:CG2  | 2.50                     | 0.40              |
| 3:D:138:LYS:CB    | 3:D:450:TYR:OH   | 2.66                     | 0.40              |
| 3:D:508:ARG:HA    | 3:D:509:PRO:HD2  | 1.80                     | 0.40              |
| 3:D:508:ARG:HB2   | 3:D:511:TRP:NE1  | 2.36                     | 0.40              |
| 3:D:87:ARG:O      | 3:D:524:LEU:HD11 | 2.22                     | 0.40              |
| 3:D:564:GLU:HA    | 3:D:567:ILE:CG1  | 2.51                     | 0.40              |
| 3:D:654:LYS:HD3   | 3:D:655:PRO:HD3  | 2.03                     | 0.40              |
| 3:D:681:ARG:HG3   | 3:D:682:ASP:OD1  | 2.21                     | 0.40              |
| 3:D:934:LEU:O     | 3:D:935:LYS:C    | 2.59                     | 0.40              |
| 2:C:987:ILE:CG2   | 3:D:948:THR:HG21 | 2.52                     | 0.40              |
| 5:F:181:GLU:OE2   | 5:F:184:ARG:HD3  | 2.21                     | 0.40              |
| 5:F:189:GLU:O     | 5:F:191:ASN:N    | 2.55                     | 0.40              |
| 5:F:260:ILE:CG1   | 5:F:261:PRO:HD2  | 2.51                     | 0.40              |
| 5:F:381:HIS:HB3   | 5:F:384:GLU:CG   | 2.51                     | 0.40              |
| 1:K:111:ALA:C     | 1:K:113:ASP:H    | 2.23                     | 0.40              |
| 1:L:137:ARG:HH22  | 1:L:139:ASN:HD22 | 1.69                     | 0.40              |
| 1:L:208:LEU:HD11  | 1:L:212:ASN:HD21 | 1.85                     | 0.40              |
| 2:M:212:GLY:O     | 2:M:215:GLY:C    | 2.59                     | 0.40              |
| 2:M:446:GLY:O     | 2:M:449:ILE:HG22 | 2.22                     | 0.40              |
| 2:M:397:GLU:CD    | 2:M:632:ASN:H    | 2.23                     | 0.40              |
| 2:M:728:HIS:HD2   | 2:M:734:LEU:HD21 | 1.87                     | 0.40              |
| 2:M:890:LEU:O     | 2:M:891:GLY:C    | 2.59                     | 0.40              |
| 2:M:909:ALA:C     | 2:M:910:LYS:HD2  | 2.41                     | 0.40              |
| 3:N:116:LEU:HB2   | 3:N:118:LEU:HG   | 2.03                     | 0.40              |
| 3:N:119:SER:CB    | 3:N:123:LEU:H    | 2.25                     | 0.40              |
| 3:N:1283:ILE:HD12 | 3:N:1315:ASP:OD2 | 2.22                     | 0.40              |
| 3:N:1292:VAL:CG1  | 3:N:1293:PHE:N   | 2.82                     | 0.40              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1462:LEU:HB3  | 3:N:1472:ILE:CD1  | 2.52                     | 0.40              |
| 3:N:149:LYS:CG    | 3:N:150:ARG:H     | 2.30                     | 0.40              |
| 3:N:259:VAL:HG11  | 3:N:293:VAL:HG12  | 2.02                     | 0.40              |
| 3:N:34:TYR:CG     | 3:N:35:ARG:N      | 2.89                     | 0.40              |
| 3:N:416:ALA:CB    | 3:N:432:TYR:CA    | 2.84                     | 0.40              |
| 3:N:645:PRO:O     | 3:N:646:LYS:C     | 2.60                     | 0.40              |
| 3:N:784:ASP:OD1   | 3:N:784:ASP:N     | 2.50                     | 0.40              |
| 3:N:806:PHE:CE2   | 3:N:809:PRO:C     | 2.95                     | 0.40              |
| 3:N:933:ALA:O     | 3:N:936:TYR:HB3   | 2.20                     | 0.40              |
| 5:P:215:GLU:O     | 5:P:218:GLN:CG    | 2.68                     | 0.40              |
| 5:P:321:ILE:HG22  | 5:P:322:GLY:N     | 2.37                     | 0.40              |
| 5:P:320:PRO:HA    | 5:P:327:SER:O     | 2.20                     | 0.40              |
| 5:P:329:TYR:O     | 5:P:330:GLY:C     | 2.60                     | 0.40              |
| 5:P:405:LEU:O     | 5:P:408:LEU:HB3   | 2.21                     | 0.40              |
| 1:B:112:ARG:CG    | 1:B:113:ASP:H     | 2.35                     | 0.40              |
| 1:B:211:LEU:HD12  | 1:B:211:LEU:C     | 2.42                     | 0.40              |
| 2:C:173:ASP:O     | 2:C:174:LEU:HD23  | 2.21                     | 0.40              |
| 2:C:300:ASP:OD2   | 2:C:303:PHE:CD1   | 2.74                     | 0.40              |
| 2:C:110:GLU:CG    | 2:C:369:PRO:HB3   | 2.50                     | 0.40              |
| 2:C:571:LEU:HD12  | 2:C:670:GLN:HG3   | 2.04                     | 0.40              |
| 2:C:598:GLU:H     | 2:C:598:GLU:HG2   | 1.66                     | 0.40              |
| 2:C:630:ARG:HH11  | 2:C:630:ARG:HG2   | 1.86                     | 0.40              |
| 2:C:694:LEU:HD23  | 2:C:697:ARG:NH2   | 2.36                     | 0.40              |
| 2:C:723:THR:OG1   | 2:C:725:ASP:HB3   | 2.21                     | 0.40              |
| 2:C:726:ILE:C     | 2:C:728:HIS:N     | 2.73                     | 0.40              |
| 2:C:806:LEU:O     | 2:C:821:GLU:HB2   | 2.21                     | 0.40              |
| 2:C:841:ASN:C     | 2:C:843:HIS:H     | 2.23                     | 0.40              |
| 2:C:860:HIS:NE2   | 2:C:975:TYR:HB2   | 2.36                     | 0.40              |
| 2:C:965:GLU:O     | 2:C:969:GLN:HG3   | 2.22                     | 0.40              |
| 3:D:1008:PHE:CD1  | 3:D:1008:PHE:N    | 2.89                     | 0.40              |
| 3:D:1032:PRO:O    | 3:D:1033:GLN:C    | 2.60                     | 0.40              |
| 3:D:1047:LYS:HD2  | 3:D:1051:GLU:HG3  | 2.03                     | 0.40              |
| 3:D:1262:LEU:HD13 | 3:D:1352:ILE:HG13 | 2.04                     | 0.40              |
| 3:D:1280:VAL:CG1  | 3:D:1316:GLY:HA2  | 2.52                     | 0.40              |
| 3:D:1453:ALA:O    | 3:D:1454:GLY:C    | 2.59                     | 0.40              |
| 3:D:139:GLY:HA3   | 3:D:147:VAL:HG23  | 2.02                     | 0.40              |
| 3:D:283:PHE:CE2   | 3:D:313:MET:SD    | 3.14                     | 0.40              |
| 3:D:209:ARG:HB2   | 3:D:389:GLU:CB    | 2.51                     | 0.40              |
| 3:D:517:VAL:HA    | 3:D:518:PRO:HD3   | 1.83                     | 0.40              |
| 3:D:627:GLY:O     | 3:D:747:VAL:HG12  | 2.21                     | 0.40              |
| 2:M:1064:ASN:O    | 2:M:1065:ALA:C    | 2.59                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:19:THR:O      | 2:M:23:VAL:HG22  | 2.20                     | 0.40              |
| 2:M:18:LEU:HD12   | 2:M:590:ASP:CB   | 2.52                     | 0.40              |
| 2:M:953:VAL:HG11  | 2:M:962:GLN:HB3  | 2.03                     | 0.40              |
| 3:N:1067:VAL:HG13 | 3:N:1068:LEU:N   | 2.33                     | 0.40              |
| 3:N:133:ILE:HG22  | 3:N:455:ARG:CA   | 2.51                     | 0.40              |
| 3:N:1351:GLU:OE2  | 3:N:1354:LYS:HD2 | 2.20                     | 0.40              |
| 3:N:247:GLU:HA    | 3:N:248:PRO:HA   | 1.80                     | 0.40              |
| 3:N:32:ILE:HG23   | 3:N:38:LYS:N     | 2.36                     | 0.40              |
| 3:N:409:VAL:HG12  | 3:N:410:SER:H    | 1.85                     | 0.40              |
| 3:N:416:ALA:HB1   | 3:N:432:TYR:CD1  | 2.56                     | 0.40              |
| 3:N:543:LEU:HA    | 3:N:546:ARG:HD3  | 2.03                     | 0.40              |
| 3:N:564:GLU:O     | 3:N:565:ILE:C    | 2.59                     | 0.40              |
| 3:N:657:LEU:HG    | 3:N:661:MET:HE3  | 2.04                     | 0.40              |
| 3:N:662:GLU:N     | 3:N:667:ALA:HB3  | 2.36                     | 0.40              |
| 3:N:66:GLN:O      | 3:N:66:GLN:HG2   | 2.21                     | 0.40              |
| 3:N:827:ILE:HA    | 3:N:836:VAL:CB   | 2.34                     | 0.40              |
| 3:N:956:ILE:HA    | 3:N:957:PRO:HD3  | 1.90                     | 0.40              |
| 3:N:989:TYR:CD1   | 3:N:993:LEU:HD21 | 2.57                     | 0.40              |
| 5:P:328:PHE:O     | 5:P:332:PHE:CE1  | 2.74                     | 0.40              |
| 5:P:402:ASN:ND2   | 5:P:402:ASN:N    | 2.70                     | 0.40              |
| 1:A:133:GLU:CG    | 1:A:134:GLU:N    | 2.85                     | 0.40              |
| 1:A:155:LYS:HB3   | 1:A:156:HIS:H    | 1.73                     | 0.40              |
| 1:A:220:GLU:O     | 1:A:224:TYR:CE2  | 2.73                     | 0.40              |
| 1:B:184:THR:HG23  | 1:B:192:LEU:HB2  | 2.04                     | 0.40              |
| 2:C:185:LYS:HE2   | 2:C:190:LYS:HD3  | 2.03                     | 0.40              |
| 2:C:217:LEU:C     | 2:C:219:GLN:H    | 2.24                     | 0.40              |
| 2:C:359:MET:HG2   | 2:C:359:MET:O    | 2.22                     | 0.40              |
| 2:C:343:GLN:CG    | 2:C:385:PHE:HB2  | 2.50                     | 0.40              |
| 2:C:385:PHE:O     | 2:C:389:SER:N    | 2.54                     | 0.40              |
| 2:C:612:VAL:HG13  | 2:C:622:GLU:CA   | 2.51                     | 0.40              |
| 2:C:860:HIS:HA    | 2:C:866:PRO:HA   | 2.03                     | 0.40              |
| 2:C:910:LYS:O     | 2:C:911:GLU:C    | 2.60                     | 0.40              |
| 3:D:1025:GLN:C    | 3:D:1027:GLY:H   | 2.24                     | 0.40              |
| 3:D:1042:ARG:HH11 | 3:D:1042:ARG:CG  | 2.31                     | 0.40              |
| 3:D:1055:VAL:HA   | 3:D:1056:PRO:HD3 | 1.90                     | 0.40              |
| 3:D:1066:THR:HB   | 3:D:1069:GLU:CG  | 2.51                     | 0.40              |
| 3:D:1092:GLY:O    | 3:D:1095:THR:N   | 2.55                     | 0.40              |
| 3:D:1103:HIS:HD2  | 3:D:1462:LEU:CB  | 2.35                     | 0.40              |
| 3:D:148:GLU:C     | 3:D:150:ARG:N    | 2.74                     | 0.40              |
| 3:D:148:GLU:O     | 3:D:150:ARG:N    | 2.55                     | 0.40              |
| 3:D:15:PRO:O      | 3:D:18:ILE:HB    | 2.20                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:245:LEU:CA   | 3:D:309:GLY:H    | 2.32                     | 0.40              |
| 3:D:462:GLN:O    | 3:D:463:GLN:C    | 2.59                     | 0.40              |
| 3:D:520:LEU:HD11 | 3:D:524:LEU:CD1  | 2.51                     | 0.40              |
| 3:D:670:VAL:O    | 3:D:671:LYS:C    | 2.60                     | 0.40              |
| 3:D:686:GLU:O    | 3:D:687:VAL:C    | 2.59                     | 0.40              |
| 3:D:764:LEU:HD23 | 3:D:767:HIS:CD2  | 2.56                     | 0.40              |
| 3:D:806:PHE:CE2  | 3:D:812:ALA:HB2  | 2.57                     | 0.40              |
| 2:C:1018:GLN:HG2 | 3:D:87:ARG:NH2   | 2.37                     | 0.40              |
| 3:D:932:ASP:O    | 3:D:933:ALA:C    | 2.60                     | 0.40              |
| 3:D:95:LEU:HB2   | 3:D:515:GLU:CA   | 2.41                     | 0.40              |
| 3:D:95:LEU:HD21  | 3:D:517:VAL:CG2  | 2.52                     | 0.40              |
| 4:E:29:GLN:C     | 4:E:31:LEU:N     | 2.75                     | 0.40              |
| 5:F:102:LEU:HD12 | 5:F:183:ALA:HB1  | 2.04                     | 0.40              |
| 5:F:125:ASP:CG   | 5:F:126:LEU:H    | 2.25                     | 0.40              |
| 5:F:148:LYS:O    | 5:F:149:GLU:C    | 2.60                     | 0.40              |
| 5:F:102:LEU:HD11 | 5:F:183:ALA:HA   | 2.04                     | 0.40              |
| 5:F:289:GLU:O    | 5:F:290:GLU:C    | 2.59                     | 0.40              |
| 5:F:314:PRO:CG   | 5:F:315:VAL:N    | 2.79                     | 0.40              |
| 5:F:381:HIS:HB3  | 5:F:384:GLU:CD   | 2.42                     | 0.40              |
| 1:K:22:GLU:C     | 1:K:23:PHE:CD1   | 2.95                     | 0.40              |
| 1:L:86:VAL:HG12  | 1:L:124:ASN:ND2  | 2.36                     | 0.40              |
| 2:M:1048:THR:HA  | 3:N:755:ALA:CB   | 2.51                     | 0.40              |
| 2:M:129:ILE:N    | 2:M:129:ILE:HD13 | 2.37                     | 0.40              |
| 2:M:280:LYS:O    | 2:M:281:LEU:HD23 | 2.20                     | 0.40              |
| 2:M:512:ARG:HH11 | 2:M:524:VAL:HA   | 1.86                     | 0.40              |
| 2:M:649:VAL:CG1  | 2:M:650:ARG:HH21 | 2.33                     | 0.40              |
| 2:M:809:GLY:O    | 2:M:813:VAL:HB   | 2.21                     | 0.40              |
| 2:M:86:LYS:O     | 2:M:87:ASP:C     | 2.60                     | 0.40              |
| 2:M:941:VAL:O    | 2:M:944:LEU:HB2  | 2.22                     | 0.40              |
| 2:M:958:THR:O    | 2:M:962:GLN:HG3  | 2.21                     | 0.40              |
| 3:N:134:VAL:HG12 | 3:N:136:ASP:OD1  | 2.22                     | 0.40              |
| 3:N:206:ARG:NE   | 3:N:392:SER:CB   | 2.82                     | 0.40              |
| 3:N:221:ALA:O    | 3:N:334:THR:HA   | 2.20                     | 0.40              |
| 3:N:358:GLY:HA2  | 3:N:385:VAL:O    | 2.22                     | 0.40              |
| 3:N:541:ASN:O    | 3:N:544:TYR:HB2  | 2.22                     | 0.40              |
| 3:N:60:CYS:SG    | 3:N:62:LYS:HE2   | 2.61                     | 0.40              |
| 3:N:680:GLN:O    | 3:N:683:ILE:HB   | 2.22                     | 0.40              |
| 3:N:5:VAL:CG1    | 3:N:6:ARG:N      | 2.84                     | 0.40              |
| 3:N:73:CYS:C     | 3:N:75:ARG:N     | 2.75                     | 0.40              |
| 3:N:871:LYS:NZ   | 3:N:897:TRP:CH2  | 2.89                     | 0.40              |
| 3:N:984:THR:O    | 3:N:987:GLU:HB2  | 2.21                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 5:P:102:LEU:HD21 | 5:P:187:LEU:HB2 | 2.03                     | 0.40              |
| 5:P:239:ALA:O    | 5:P:241:TRP:N   | 2.54                     | 0.40              |
| 5:P:315:VAL:HG12 | 5:P:316:SER:N   | 2.36                     | 0.40              |
| 5:P:353:GLU:HA   | 5:P:356:LYS:CB  | 2.51                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed    | Outliers  | Percentiles |    |
|-----|-------|------------------|------------|------------|-----------|-------------|----|
| 1   | A     | 229/315 (73%)    | 160 (70%)  | 54 (24%)   | 15 (7%)   | 1           | 6  |
| 1   | B     | 241/315 (76%)    | 159 (66%)  | 64 (27%)   | 18 (8%)   | 1           | 5  |
| 1   | K     | 229/315 (73%)    | 168 (73%)  | 50 (22%)   | 11 (5%)   | 2           | 13 |
| 1   | L     | 241/315 (76%)    | 171 (71%)  | 55 (23%)   | 15 (6%)   | 1           | 8  |
| 2   | C     | 1117/1119 (100%) | 774 (69%)  | 251 (22%)  | 92 (8%)   | 1           | 4  |
| 2   | M     | 1117/1119 (100%) | 767 (69%)  | 246 (22%)  | 104 (9%)  | 0           | 3  |
| 3   | D     | 1502/1524 (99%)  | 931 (62%)  | 422 (28%)  | 149 (10%) | 0           | 2  |
| 3   | N     | 1502/1524 (99%)  | 907 (60%)  | 445 (30%)  | 150 (10%) | 0           | 2  |
| 4   | E     | 93/99 (94%)      | 54 (58%)   | 25 (27%)   | 14 (15%)  | 0           | 1  |
| 4   | O     | 93/99 (94%)      | 56 (60%)   | 27 (29%)   | 10 (11%)  | 0           | 2  |
| 5   | F     | 347/423 (82%)    | 167 (48%)  | 130 (38%)  | 50 (14%)  | 0           | 1  |
| 5   | P     | 347/423 (82%)    | 171 (49%)  | 117 (34%)  | 59 (17%)  | 0           | 0  |
| All | All   | 7058/7590 (93%)  | 4485 (64%) | 1886 (27%) | 687 (10%) | 0           | 2  |

All (687) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 59   | GLU  |
| 1   | A     | 112  | ARG  |
| 1   | A     | 155  | LYS  |
| 1   | B     | 75   | VAL  |
| 1   | B     | 118  | ALA  |
| 2   | C     | 33   | ASP  |
| 2   | C     | 42   | VAL  |
| 2   | C     | 113  | VAL  |
| 2   | C     | 272  | ALA  |
| 2   | C     | 276  | LYS  |
| 2   | C     | 294  | GLU  |
| 2   | C     | 368  | THR  |
| 2   | C     | 385  | PHE  |
| 2   | C     | 399  | ASN  |
| 2   | C     | 909  | ALA  |
| 2   | C     | 984  | GLU  |
| 2   | C     | 1060 | ILE  |
| 3   | D     | 111  | LYS  |
| 3   | D     | 137  | PRO  |
| 3   | D     | 248  | PRO  |
| 3   | D     | 292  | VAL  |
| 3   | D     | 485  | SER  |
| 3   | D     | 487  | ALA  |
| 3   | D     | 545  | ARG  |
| 3   | D     | 607  | LEU  |
| 3   | D     | 751  | LEU  |
| 3   | D     | 836  | VAL  |
| 3   | D     | 908  | LYS  |
| 3   | D     | 945  | SER  |
| 3   | D     | 1074 | SER  |
| 3   | D     | 1342 | GLU  |
| 3   | D     | 1366 | LYS  |
| 3   | D     | 1405 | GLU  |
| 3   | D     | 1426 | LYS  |
| 3   | D     | 1427 | SER  |
| 3   | D     | 1446 | VAL  |
| 4   | E     | 22   | VAL  |
| 4   | E     | 38   | THR  |
| 4   | E     | 87   | LYS  |
| 5   | F     | 75   | ILE  |
| 5   | F     | 100  | VAL  |
| 5   | F     | 116  | LEU  |
| 5   | F     | 188  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | F     | 314  | PRO  |
| 5   | F     | 363  | GLU  |
| 5   | F     | 402  | ASN  |
| 1   | K     | 73   | GLU  |
| 1   | L     | 59   | GLU  |
| 1   | L     | 240  | LYS  |
| 2   | M     | 21   | ILE  |
| 2   | M     | 33   | ASP  |
| 2   | M     | 42   | VAL  |
| 2   | M     | 178  | PRO  |
| 2   | M     | 183  | SER  |
| 2   | M     | 194  | VAL  |
| 2   | M     | 255  | ALA  |
| 2   | M     | 276  | LYS  |
| 2   | M     | 542  | VAL  |
| 2   | M     | 562  | SER  |
| 2   | M     | 604  | ALA  |
| 2   | M     | 684  | PHE  |
| 2   | M     | 730  | SER  |
| 2   | M     | 782  | ALA  |
| 2   | M     | 855  | VAL  |
| 2   | M     | 909  | ALA  |
| 2   | M     | 1046 | ALA  |
| 2   | M     | 1060 | ILE  |
| 3   | N     | 46   | ASP  |
| 3   | N     | 137  | PRO  |
| 3   | N     | 149  | LYS  |
| 3   | N     | 227  | LEU  |
| 3   | N     | 245  | LEU  |
| 3   | N     | 248  | PRO  |
| 3   | N     | 292  | VAL  |
| 3   | N     | 481  | MET  |
| 3   | N     | 487  | ALA  |
| 3   | N     | 492  | ALA  |
| 3   | N     | 607  | LEU  |
| 3   | N     | 639  | LEU  |
| 3   | N     | 650  | LEU  |
| 3   | N     | 734  | GLU  |
| 3   | N     | 766  | ALA  |
| 3   | N     | 808  | THR  |
| 3   | N     | 836  | VAL  |
| 3   | N     | 908  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 936  | TYR  |
| 3   | N     | 962  | GLN  |
| 3   | N     | 989  | TYR  |
| 3   | N     | 1007 | VAL  |
| 3   | N     | 1094 | LEU  |
| 3   | N     | 1125 | PRO  |
| 3   | N     | 1405 | GLU  |
| 3   | N     | 1446 | VAL  |
| 3   | N     | 1467 | ILE  |
| 4   | O     | 16   | LYS  |
| 5   | P     | 75   | ILE  |
| 5   | P     | 78   | SER  |
| 5   | P     | 93   | LEU  |
| 5   | P     | 100  | VAL  |
| 5   | P     | 159  | ILE  |
| 5   | P     | 236  | SER  |
| 5   | P     | 331  | ASP  |
| 5   | P     | 356  | LYS  |
| 5   | P     | 363  | GLU  |
| 5   | P     | 368  | VAL  |
| 5   | P     | 376  | ILE  |
| 5   | P     | 400  | ILE  |
| 5   | P     | 402  | ASN  |
| 1   | A     | 32   | PHE  |
| 1   | A     | 35   | THR  |
| 1   | A     | 47   | SER  |
| 1   | A     | 217  | ILE  |
| 1   | B     | 113  | ASP  |
| 2   | C     | 21   | ILE  |
| 2   | C     | 80   | GLN  |
| 2   | C     | 179  | ASN  |
| 2   | C     | 212  | GLY  |
| 2   | C     | 241  | LEU  |
| 2   | C     | 251  | ASP  |
| 2   | C     | 271  | GLU  |
| 2   | C     | 284  | ARG  |
| 2   | C     | 297  | GLU  |
| 2   | C     | 336  | VAL  |
| 2   | C     | 369  | PRO  |
| 2   | C     | 381  | ALA  |
| 2   | C     | 386  | PHE  |
| 2   | C     | 447  | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 500  | ASN  |
| 2   | C     | 715  | THR  |
| 2   | C     | 809  | GLY  |
| 2   | C     | 855  | VAL  |
| 2   | C     | 856  | GLU  |
| 2   | C     | 883  | GLY  |
| 2   | C     | 927  | GLY  |
| 2   | C     | 929  | ARG  |
| 2   | C     | 1004 | LYS  |
| 2   | C     | 1115 | LEU  |
| 3   | D     | 46   | ASP  |
| 3   | D     | 65   | ARG  |
| 3   | D     | 103  | TRP  |
| 3   | D     | 120  | ALA  |
| 3   | D     | 124  | GLU  |
| 3   | D     | 126  | VAL  |
| 3   | D     | 227  | LEU  |
| 3   | D     | 246  | PRO  |
| 3   | D     | 457  | GLY  |
| 3   | D     | 564  | GLU  |
| 3   | D     | 565  | ILE  |
| 3   | D     | 666  | ILE  |
| 3   | D     | 676  | MET  |
| 3   | D     | 686  | GLU  |
| 3   | D     | 737  | ASN  |
| 3   | D     | 752  | SER  |
| 3   | D     | 759  | ALA  |
| 3   | D     | 808  | THR  |
| 3   | D     | 809  | PRO  |
| 3   | D     | 811  | GLU  |
| 3   | D     | 813  | LEU  |
| 3   | D     | 885  | ILE  |
| 3   | D     | 894  | LYS  |
| 3   | D     | 923  | GLY  |
| 3   | D     | 962  | GLN  |
| 3   | D     | 966  | GLU  |
| 3   | D     | 1007 | VAL  |
| 3   | D     | 1071 | PHE  |
| 3   | D     | 1072 | ILE  |
| 3   | D     | 1263 | PHE  |
| 3   | D     | 1316 | GLY  |
| 3   | D     | 1338 | ALA  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1341 | PRO  |
| 3   | D     | 1347 | TYR  |
| 3   | D     | 1354 | LYS  |
| 3   | D     | 1367 | HIS  |
| 3   | D     | 1384 | PRO  |
| 3   | D     | 1467 | ILE  |
| 3   | D     | 1482 | ARG  |
| 4   | E     | 21   | VAL  |
| 4   | E     | 71   | GLY  |
| 4   | E     | 85   | LEU  |
| 5   | F     | 77   | THR  |
| 5   | F     | 78   | SER  |
| 5   | F     | 81   | VAL  |
| 5   | F     | 93   | LEU  |
| 5   | F     | 119  | ILE  |
| 5   | F     | 127  | ILE  |
| 5   | F     | 131  | VAL  |
| 5   | F     | 132  | ARG  |
| 5   | F     | 195  | VAL  |
| 5   | F     | 205  | ARG  |
| 5   | F     | 236  | SER  |
| 5   | F     | 238  | TYR  |
| 5   | F     | 266  | GLU  |
| 5   | F     | 288  | TYR  |
| 5   | F     | 304  | VAL  |
| 5   | F     | 351  | SER  |
| 5   | F     | 404  | ALA  |
| 1   | K     | 5    | LYS  |
| 1   | K     | 59   | GLU  |
| 1   | L     | 37   | GLY  |
| 1   | L     | 118  | ALA  |
| 2   | M     | 20   | GLU  |
| 2   | M     | 38   | LYS  |
| 2   | M     | 49   | ARG  |
| 2   | M     | 80   | GLN  |
| 2   | M     | 81   | ASP  |
| 2   | M     | 111  | ASP  |
| 2   | M     | 113  | VAL  |
| 2   | M     | 152  | PRO  |
| 2   | M     | 218  | VAL  |
| 2   | M     | 314  | THR  |
| 2   | M     | 322  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 381  | ALA  |
| 2   | M     | 423  | ALA  |
| 2   | M     | 425  | PHE  |
| 2   | M     | 463  | GLU  |
| 2   | M     | 583  | LEU  |
| 2   | M     | 584  | GLU  |
| 2   | M     | 616  | GLU  |
| 2   | M     | 658  | GLY  |
| 2   | M     | 692  | GLU  |
| 2   | M     | 728  | HIS  |
| 2   | M     | 735  | ARG  |
| 2   | M     | 809  | GLY  |
| 2   | M     | 923  | GLU  |
| 2   | M     | 927  | GLY  |
| 2   | M     | 943  | VAL  |
| 2   | M     | 1050 | GLN  |
| 3   | N     | 69   | GLU  |
| 3   | N     | 111  | LYS  |
| 3   | N     | 122  | GLU  |
| 3   | N     | 124  | GLU  |
| 3   | N     | 126  | VAL  |
| 3   | N     | 146  | PRO  |
| 3   | N     | 162  | ARG  |
| 3   | N     | 358  | GLY  |
| 3   | N     | 407  | VAL  |
| 3   | N     | 442  | ASN  |
| 3   | N     | 485  | SER  |
| 3   | N     | 526  | PRO  |
| 3   | N     | 532  | GLY  |
| 3   | N     | 545  | ARG  |
| 3   | N     | 565  | ILE  |
| 3   | N     | 654  | LYS  |
| 3   | N     | 666  | ILE  |
| 3   | N     | 686  | GLU  |
| 3   | N     | 731  | LEU  |
| 3   | N     | 761  | ILE  |
| 3   | N     | 787  | LEU  |
| 3   | N     | 846  | PRO  |
| 3   | N     | 939  | PHE  |
| 3   | N     | 940  | THR  |
| 3   | N     | 945  | SER  |
| 3   | N     | 988  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1072 | ILE  |
| 3   | N     | 1082 | ALA  |
| 3   | N     | 1171 | VAL  |
| 3   | N     | 1234 | THR  |
| 3   | N     | 1341 | PRO  |
| 3   | N     | 1348 | LEU  |
| 3   | N     | 1349 | VAL  |
| 3   | N     | 1355 | VAL  |
| 3   | N     | 1366 | LYS  |
| 3   | N     | 1377 | LYS  |
| 3   | N     | 1397 | LYS  |
| 3   | N     | 1399 | ASP  |
| 3   | N     | 1424 | VAL  |
| 3   | N     | 1435 | LEU  |
| 3   | N     | 1482 | ARG  |
| 3   | N     | 1503 | VAL  |
| 3   | N     | 1504 | GLU  |
| 4   | O     | 30   | LEU  |
| 4   | O     | 71   | GLY  |
| 4   | O     | 72   | ARG  |
| 4   | O     | 82   | GLU  |
| 4   | O     | 85   | LEU  |
| 4   | O     | 87   | LYS  |
| 5   | P     | 85   | LEU  |
| 5   | P     | 155  | THR  |
| 5   | P     | 226  | LYS  |
| 5   | P     | 230  | LYS  |
| 5   | P     | 232  | ARG  |
| 5   | P     | 237  | THR  |
| 5   | P     | 238  | TYR  |
| 5   | P     | 241  | TRP  |
| 5   | P     | 247  | ILE  |
| 5   | P     | 266  | GLU  |
| 5   | P     | 271  | LEU  |
| 5   | P     | 277  | GLN  |
| 5   | P     | 288  | TYR  |
| 5   | P     | 297  | PRO  |
| 5   | P     | 307  | THR  |
| 5   | P     | 322  | GLY  |
| 5   | P     | 351  | SER  |
| 5   | P     | 352  | GLU  |
| 5   | P     | 354  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | P     | 360  | LYS  |
| 5   | P     | 382  | THR  |
| 1   | A     | 97   | VAL  |
| 1   | A     | 105  | GLY  |
| 1   | B     | 59   | GLU  |
| 1   | B     | 119  | ASP  |
| 1   | B     | 208  | LEU  |
| 2   | C     | 7    | GLY  |
| 2   | C     | 20   | GLU  |
| 2   | C     | 49   | ARG  |
| 2   | C     | 152  | PRO  |
| 2   | C     | 183  | SER  |
| 2   | C     | 222  | MET  |
| 2   | C     | 291  | ALA  |
| 2   | C     | 306  | THR  |
| 2   | C     | 400  | PRO  |
| 2   | C     | 423  | ALA  |
| 2   | C     | 463  | GLU  |
| 2   | C     | 551  | GLU  |
| 2   | C     | 772  | ARG  |
| 2   | C     | 1050 | GLN  |
| 3   | D     | 128  | TYR  |
| 3   | D     | 200  | ASP  |
| 3   | D     | 235  | ALA  |
| 3   | D     | 237  | LYS  |
| 3   | D     | 310  | LEU  |
| 3   | D     | 405  | ASP  |
| 3   | D     | 467  | GLU  |
| 3   | D     | 474  | GLU  |
| 3   | D     | 492  | ALA  |
| 3   | D     | 504  | ASP  |
| 3   | D     | 505  | SER  |
| 3   | D     | 506  | GLY  |
| 3   | D     | 523  | ASP  |
| 3   | D     | 612  | GLY  |
| 3   | D     | 617  | ASN  |
| 3   | D     | 639  | LEU  |
| 3   | D     | 684  | LYS  |
| 3   | D     | 734  | GLU  |
| 3   | D     | 760  | ARG  |
| 3   | D     | 791  | TYR  |
| 3   | D     | 846  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 902  | LEU  |
| 3   | D     | 989  | TYR  |
| 3   | D     | 1019 | PRO  |
| 3   | D     | 1125 | PRO  |
| 3   | D     | 1245 | GLY  |
| 3   | D     | 1315 | ASP  |
| 3   | D     | 1332 | PRO  |
| 3   | D     | 1397 | LYS  |
| 3   | D     | 1408 | ILE  |
| 3   | D     | 1447 | LEU  |
| 3   | D     | 1480 | PHE  |
| 4   | E     | 11   | GLY  |
| 4   | E     | 28   | GLN  |
| 4   | E     | 72   | ARG  |
| 5   | F     | 133  | ALA  |
| 5   | F     | 190  | ALA  |
| 5   | F     | 225  | GLU  |
| 5   | F     | 280  | GLN  |
| 5   | F     | 352  | GLU  |
| 5   | F     | 354  | LEU  |
| 5   | F     | 362  | SER  |
| 5   | F     | 382  | THR  |
| 5   | F     | 385  | GLU  |
| 5   | F     | 408  | LEU  |
| 1   | K     | 9    | PRO  |
| 1   | K     | 47   | SER  |
| 1   | L     | 241  | GLU  |
| 1   | L     | 242  | PRO  |
| 2   | M     | 19   | THR  |
| 2   | M     | 66   | LEU  |
| 2   | M     | 205  | GLU  |
| 2   | M     | 241  | LEU  |
| 2   | M     | 251  | ASP  |
| 2   | M     | 253  | ALA  |
| 2   | M     | 271  | GLU  |
| 2   | M     | 360  | LEU  |
| 2   | M     | 368  | THR  |
| 2   | M     | 380  | ALA  |
| 2   | M     | 386  | PHE  |
| 2   | M     | 400  | PRO  |
| 2   | M     | 447  | ALA  |
| 2   | M     | 551  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 563  | ASN  |
| 2   | M     | 606  | VAL  |
| 2   | M     | 897  | LEU  |
| 2   | M     | 944  | LEU  |
| 2   | M     | 977  | GLY  |
| 2   | M     | 1061 | GLU  |
| 3   | N     | 127  | LEU  |
| 3   | N     | 173  | PRO  |
| 3   | N     | 237  | LYS  |
| 3   | N     | 411  | THR  |
| 3   | N     | 480  | GLU  |
| 3   | N     | 549  | ASN  |
| 3   | N     | 606  | ILE  |
| 3   | N     | 655  | PRO  |
| 3   | N     | 687  | VAL  |
| 3   | N     | 737  | ASN  |
| 3   | N     | 809  | PRO  |
| 3   | N     | 1032 | PRO  |
| 3   | N     | 1224 | VAL  |
| 3   | N     | 1297 | GLU  |
| 3   | N     | 1338 | ALA  |
| 4   | O     | 59   | ASN  |
| 5   | P     | 77   | THR  |
| 5   | P     | 169  | GLU  |
| 5   | P     | 190  | ALA  |
| 5   | P     | 225  | GLU  |
| 5   | P     | 353  | GLU  |
| 1   | B     | 44   | LEU  |
| 1   | B     | 171  | PHE  |
| 1   | B     | 217  | ILE  |
| 1   | B     | 236  | PRO  |
| 2   | C     | 74   | GLY  |
| 2   | C     | 178  | PRO  |
| 2   | C     | 231  | PRO  |
| 2   | C     | 244  | PRO  |
| 2   | C     | 537  | LYS  |
| 2   | C     | 584  | GLU  |
| 2   | C     | 604  | ALA  |
| 2   | C     | 684  | PHE  |
| 2   | C     | 730  | SER  |
| 2   | C     | 876  | VAL  |
| 2   | C     | 915  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 955  | PRO  |
| 2   | C     | 1020 | PRO  |
| 3   | D     | 39   | PRO  |
| 3   | D     | 69   | GLU  |
| 3   | D     | 123  | LEU  |
| 3   | D     | 172  | PRO  |
| 3   | D     | 199  | LEU  |
| 3   | D     | 295  | GLY  |
| 3   | D     | 356  | PRO  |
| 3   | D     | 377  | VAL  |
| 3   | D     | 460  | ALA  |
| 3   | D     | 472  | ALA  |
| 3   | D     | 546  | ARG  |
| 3   | D     | 603  | LEU  |
| 3   | D     | 654  | LYS  |
| 3   | D     | 668  | PRO  |
| 3   | D     | 936  | TYR  |
| 3   | D     | 995  | LEU  |
| 3   | D     | 1023 | MET  |
| 3   | D     | 1079 | LYS  |
| 3   | D     | 1082 | ALA  |
| 3   | D     | 1093 | TYR  |
| 3   | D     | 1094 | LEU  |
| 3   | D     | 1448 | THR  |
| 3   | D     | 1484 | THR  |
| 3   | D     | 1497 | GLU  |
| 4   | E     | 20   | THR  |
| 4   | E     | 23   | VAL  |
| 4   | E     | 32   | ARG  |
| 5   | F     | 83   | GLN  |
| 5   | F     | 174  | LEU  |
| 5   | F     | 178  | ARG  |
| 5   | F     | 233  | PHE  |
| 5   | F     | 247  | ILE  |
| 5   | F     | 271  | LEU  |
| 1   | L     | 9    | PRO  |
| 1   | L     | 35   | THR  |
| 1   | L     | 102  | LYS  |
| 1   | L     | 211  | LEU  |
| 1   | L     | 217  | ILE  |
| 2   | M     | 12   | VAL  |
| 2   | M     | 170  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 171  | TRP  |
| 2   | M     | 208  | ALA  |
| 2   | M     | 212  | GLY  |
| 2   | M     | 213  | ALA  |
| 2   | M     | 231  | PRO  |
| 2   | M     | 256  | TYR  |
| 2   | M     | 305  | PRO  |
| 2   | M     | 306  | THR  |
| 2   | M     | 505  | GLY  |
| 2   | M     | 526  | PRO  |
| 2   | M     | 608  | GLY  |
| 2   | M     | 626  | ARG  |
| 2   | M     | 849  | VAL  |
| 2   | M     | 876  | VAL  |
| 2   | M     | 957  | LYS  |
| 3   | N     | 62   | LYS  |
| 3   | N     | 125  | GLN  |
| 3   | N     | 250  | LEU  |
| 3   | N     | 451  | ASP  |
| 3   | N     | 474  | GLU  |
| 3   | N     | 498  | VAL  |
| 3   | N     | 509  | PRO  |
| 3   | N     | 603  | LEU  |
| 3   | N     | 665  | GLY  |
| 3   | N     | 670  | VAL  |
| 3   | N     | 676  | MET  |
| 3   | N     | 757  | ALA  |
| 3   | N     | 995  | LEU  |
| 3   | N     | 1083 | ASP  |
| 3   | N     | 1342 | GLU  |
| 3   | N     | 1385 | GLY  |
| 3   | N     | 1391 | GLU  |
| 3   | N     | 1469 | GLY  |
| 4   | O     | 41   | GLU  |
| 4   | O     | 58   | PRO  |
| 5   | P     | 239  | ALA  |
| 5   | P     | 306  | GLU  |
| 5   | P     | 346  | THR  |
| 5   | P     | 392  | VAL  |
| 5   | P     | 405  | LEU  |
| 5   | P     | 420  | ASP  |
| 1   | A     | 4    | SER  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 9    | PRO  |
| 1   | A     | 30   | ARG  |
| 1   | A     | 208  | LEU  |
| 1   | B     | 35   | THR  |
| 1   | B     | 240  | LYS  |
| 2   | C     | 153  | ALA  |
| 2   | C     | 180  | GLY  |
| 2   | C     | 250  | ARG  |
| 2   | C     | 794  | PRO  |
| 2   | C     | 1061 | GLU  |
| 2   | C     | 1067 | TYR  |
| 3   | D     | 31   | THR  |
| 3   | D     | 114  | THR  |
| 3   | D     | 125  | GLN  |
| 3   | D     | 127  | LEU  |
| 3   | D     | 136  | ASP  |
| 3   | D     | 150  | ARG  |
| 3   | D     | 459  | GLU  |
| 3   | D     | 498  | VAL  |
| 3   | D     | 526  | PRO  |
| 3   | D     | 578  | VAL  |
| 3   | D     | 587  | ARG  |
| 3   | D     | 597  | ASP  |
| 3   | D     | 655  | PRO  |
| 3   | D     | 678  | GLU  |
| 3   | D     | 693  | GLU  |
| 3   | D     | 920  | LEU  |
| 3   | D     | 990  | ASP  |
| 3   | D     | 1029 | ARG  |
| 3   | D     | 1441 | GLN  |
| 3   | D     | 1445 | HIS  |
| 5   | F     | 156  | VAL  |
| 5   | F     | 213  | ILE  |
| 5   | F     | 270  | LYS  |
| 5   | F     | 272  | SER  |
| 5   | F     | 368  | VAL  |
| 1   | K     | 30   | ARG  |
| 1   | K     | 42   | ARG  |
| 2   | M     | 23   | VAL  |
| 2   | M     | 188  | LYS  |
| 2   | M     | 244  | PRO  |
| 2   | M     | 272  | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 336  | VAL  |
| 2   | M     | 510  | ALA  |
| 2   | M     | 911  | GLU  |
| 2   | M     | 1063 | ARG  |
| 3   | N     | 70   | GLY  |
| 3   | N     | 123  | LEU  |
| 3   | N     | 180  | LYS  |
| 3   | N     | 286  | VAL  |
| 3   | N     | 493  | ARG  |
| 3   | N     | 494  | LYS  |
| 3   | N     | 515  | GLU  |
| 3   | N     | 789  | LEU  |
| 3   | N     | 896  | ALA  |
| 3   | N     | 1265 | ALA  |
| 3   | N     | 1271 | LYS  |
| 3   | N     | 1332 | PRO  |
| 3   | N     | 1426 | LYS  |
| 3   | N     | 1429 | LEU  |
| 3   | N     | 1444 | THR  |
| 3   | N     | 1468 | LEU  |
| 5   | P     | 94   | LEU  |
| 5   | P     | 133  | ALA  |
| 5   | P     | 153  | PRO  |
| 1   | B     | 38   | ASN  |
| 1   | B     | 112  | ARG  |
| 1   | B     | 209  | GLU  |
| 2   | C     | 19   | THR  |
| 2   | C     | 188  | LYS  |
| 2   | C     | 248  | PRO  |
| 2   | C     | 253  | ALA  |
| 2   | C     | 304  | LEU  |
| 2   | C     | 376  | ARG  |
| 2   | C     | 658  | GLY  |
| 2   | C     | 911  | GLU  |
| 3   | D     | 412  | GLY  |
| 3   | D     | 592  | THR  |
| 3   | D     | 1097 | LYS  |
| 3   | D     | 1129 | THR  |
| 3   | D     | 1340 | GLY  |
| 5   | F     | 241  | TRP  |
| 5   | F     | 322  | GLY  |
| 1   | L     | 6    | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L     | 38   | ASN  |
| 1   | L     | 210  | ALA  |
| 2   | M     | 10   | ARG  |
| 2   | M     | 166  | PRO  |
| 2   | M     | 304  | LEU  |
| 2   | M     | 457  | ALA  |
| 2   | M     | 545  | ASN  |
| 2   | M     | 801  | VAL  |
| 2   | M     | 1062 | GLY  |
| 2   | M     | 1087 | VAL  |
| 3   | N     | 226  | PRO  |
| 3   | N     | 356  | PRO  |
| 3   | N     | 504  | ASP  |
| 3   | N     | 530  | VAL  |
| 3   | N     | 880  | ILE  |
| 3   | N     | 1040 | GLY  |
| 3   | N     | 1097 | LYS  |
| 3   | N     | 1233 | GLY  |
| 3   | N     | 1245 | GLY  |
| 3   | N     | 1414 | PRO  |
| 3   | N     | 1472 | ILE  |
| 5   | P     | 81   | VAL  |
| 5   | P     | 289  | GLU  |
| 5   | P     | 419  | ARG  |
| 2   | C     | 727  | PRO  |
| 3   | D     | 225  | LEU  |
| 3   | D     | 297  | ILE  |
| 3   | D     | 567  | ILE  |
| 3   | D     | 594  | PRO  |
| 3   | D     | 665  | GLY  |
| 3   | D     | 1003 | VAL  |
| 3   | D     | 1466 | VAL  |
| 2   | M     | 727  | PRO  |
| 3   | N     | 287  | GLY  |
| 3   | N     | 295  | GLY  |
| 3   | N     | 548  | ILE  |
| 3   | N     | 955  | VAL  |
| 3   | N     | 1003 | VAL  |
| 3   | N     | 1022 | VAL  |
| 3   | N     | 1183 | ILE  |
| 3   | N     | 1413 | THR  |
| 1   | A     | 37   | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 215  | VAL  |
| 1   | B     | 71   | VAL  |
| 2   | C     | 191  | PHE  |
| 2   | C     | 812  | GLY  |
| 3   | D     | 409  | VAL  |
| 4   | E     | 6    | ILE  |
| 5   | F     | 400  | ILE  |
| 3   | N     | 1248 | GLY  |
| 5   | P     | 146  | GLY  |
| 5   | P     | 196  | VAL  |
| 5   | P     | 251  | ILE  |
| 1   | B     | 13   | VAL  |
| 2   | C     | 165  | LEU  |
| 2   | C     | 218  | VAL  |
| 2   | C     | 542  | VAL  |
| 2   | C     | 801  | VAL  |
| 2   | C     | 844  | GLY  |
| 2   | C     | 924  | VAL  |
| 2   | C     | 931  | GLY  |
| 1   | K     | 37   | GLY  |
| 1   | K     | 43   | ILE  |
| 2   | M     | 74   | GLY  |
| 2   | M     | 794  | PRO  |
| 3   | N     | 39   | PRO  |
| 3   | N     | 85   | VAL  |
| 3   | N     | 612  | GLY  |
| 3   | N     | 788  | GLY  |
| 3   | N     | 1223 | ILE  |
| 3   | N     | 1466 | VAL  |
| 5   | P     | 188  | ILE  |
| 5   | P     | 261  | PRO  |
| 5   | P     | 313  | GLU  |
| 1   | B     | 170  | VAL  |
| 2   | C     | 505  | GLY  |
| 2   | C     | 521  | PRO  |
| 2   | C     | 526  | PRO  |
| 2   | C     | 606  | VAL  |
| 3   | D     | 786  | ILE  |
| 3   | D     | 1349 | VAL  |
| 5   | F     | 113  | ILE  |
| 5   | F     | 376  | ILE  |
| 1   | K     | 97   | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L     | 157  | GLY  |
| 2   | M     | 645  | VAL  |
| 2   | M     | 659  | PRO  |
| 3   | N     | 188  | GLY  |
| 3   | N     | 1019 | PRO  |
| 3   | N     | 1277 | ILE  |
| 5   | P     | 304  | VAL  |
| 2   | C     | 302  | VAL  |
| 4   | E     | 5    | GLY  |
| 1   | K     | 75   | VAL  |
| 2   | M     | 376  | ARG  |
| 3   | N     | 885  | ILE  |
| 3   | N     | 1394 | VAL  |
| 5   | P     | 268  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 202/273 (74%)   | 192 (95%)  | 10 (5%)   | 24          | 60 |
| 1   | B     | 210/273 (77%)   | 193 (92%)  | 17 (8%)   | 11          | 40 |
| 1   | K     | 202/273 (74%)   | 190 (94%)  | 12 (6%)   | 19          | 54 |
| 1   | L     | 210/273 (77%)   | 196 (93%)  | 14 (7%)   | 16          | 49 |
| 2   | C     | 941/941 (100%)  | 863 (92%)  | 78 (8%)   | 11          | 39 |
| 2   | M     | 941/941 (100%)  | 859 (91%)  | 82 (9%)   | 10          | 37 |
| 3   | D     | 1264/1279 (99%) | 1152 (91%) | 112 (9%)  | 9           | 35 |
| 3   | N     | 1264/1279 (99%) | 1141 (90%) | 123 (10%) | 8           | 31 |
| 4   | E     | 83/87 (95%)     | 76 (92%)   | 7 (8%)    | 11          | 38 |
| 4   | O     | 83/87 (95%)     | 74 (89%)   | 9 (11%)   | 6           | 26 |
| 5   | F     | 304/371 (82%)   | 274 (90%)  | 30 (10%)  | 8           | 30 |
| 5   | P     | 304/371 (82%)   | 266 (88%)  | 38 (12%)  | 4           | 20 |
| All | All   | 6008/6448 (93%) | 5476 (91%) | 532 (9%)  | 9           | 35 |

All (532) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | ASP  |
| 1   | A     | 23  | PHE  |
| 1   | A     | 47  | SER  |
| 1   | A     | 83  | LYS  |
| 1   | A     | 86  | VAL  |
| 1   | A     | 94  | LEU  |
| 1   | A     | 107 | LYS  |
| 1   | A     | 123 | MET  |
| 1   | A     | 124 | ASN  |
| 1   | A     | 224 | TYR  |
| 1   | B     | 23  | PHE  |
| 1   | B     | 58  | ILE  |
| 1   | B     | 82  | LEU  |
| 1   | B     | 112 | ARG  |
| 1   | B     | 113 | ASP  |
| 1   | B     | 114 | PHE  |
| 1   | B     | 124 | ASN  |
| 1   | B     | 140 | MET  |
| 1   | B     | 143 | ARG  |
| 1   | B     | 175 | ARG  |
| 1   | B     | 180 | GLN  |
| 1   | B     | 183 | ASP  |
| 1   | B     | 188 | GLN  |
| 1   | B     | 211 | LEU  |
| 1   | B     | 212 | ASN  |
| 1   | B     | 224 | TYR  |
| 1   | B     | 243 | GLU  |
| 2   | C     | 1   | MET  |
| 2   | C     | 13  | ILE  |
| 2   | C     | 15  | LEU  |
| 2   | C     | 41  | ASN  |
| 2   | C     | 71  | TYR  |
| 2   | C     | 73  | LEU  |
| 2   | C     | 81  | ASP  |
| 2   | C     | 113 | VAL  |
| 2   | C     | 115 | LEU  |
| 2   | C     | 117 | HIS  |
| 2   | C     | 139 | GLN  |
| 2   | C     | 158 | TYR  |
| 2   | C     | 179 | ASN  |
| 2   | C     | 184 | MET  |
| 2   | C     | 195 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 221 | LEU  |
| 2   | C     | 227 | PHE  |
| 2   | C     | 229 | MET  |
| 2   | C     | 230 | ARG  |
| 2   | C     | 233 | GLU  |
| 2   | C     | 239 | PHE  |
| 2   | C     | 251 | ASP  |
| 2   | C     | 263 | ASP  |
| 2   | C     | 267 | TYR  |
| 2   | C     | 268 | ASP  |
| 2   | C     | 285 | LEU  |
| 2   | C     | 303 | PHE  |
| 2   | C     | 321 | GLU  |
| 2   | C     | 361 | MET  |
| 2   | C     | 367 | LEU  |
| 2   | C     | 388 | ARG  |
| 2   | C     | 405 | ARG  |
| 2   | C     | 408 | ARG  |
| 2   | C     | 434 | HIS  |
| 2   | C     | 463 | GLU  |
| 2   | C     | 507 | ARG  |
| 2   | C     | 520 | GLU  |
| 2   | C     | 566 | THR  |
| 2   | C     | 579 | VAL  |
| 2   | C     | 584 | GLU  |
| 2   | C     | 590 | ASP  |
| 2   | C     | 600 | ASP  |
| 2   | C     | 607 | ASP  |
| 2   | C     | 610 | ARG  |
| 2   | C     | 616 | GLU  |
| 2   | C     | 622 | GLU  |
| 2   | C     | 628 | PHE  |
| 2   | C     | 630 | ARG  |
| 2   | C     | 632 | ASN  |
| 2   | C     | 650 | ARG  |
| 2   | C     | 672 | VAL  |
| 2   | C     | 674 | VAL  |
| 2   | C     | 676 | ILE  |
| 2   | C     | 680 | ASP  |
| 2   | C     | 683 | ASN  |
| 2   | C     | 699 | PHE  |
| 2   | C     | 720 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 723  | THR  |
| 2   | C     | 731  | GLU  |
| 2   | C     | 738  | ASP  |
| 2   | C     | 749  | VAL  |
| 2   | C     | 761  | PHE  |
| 2   | C     | 787  | ASP  |
| 2   | C     | 826  | TYR  |
| 2   | C     | 857  | ASP  |
| 2   | C     | 861  | LEU  |
| 2   | C     | 879  | ARG  |
| 2   | C     | 881  | ASN  |
| 2   | C     | 916  | GLU  |
| 2   | C     | 953  | VAL  |
| 2   | C     | 958  | THR  |
| 2   | C     | 1003 | ASP  |
| 2   | C     | 1020 | PRO  |
| 2   | C     | 1035 | MET  |
| 2   | C     | 1048 | THR  |
| 2   | C     | 1051 | GLU  |
| 2   | C     | 1099 | VAL  |
| 2   | C     | 1101 | THR  |
| 3   | D     | 16   | GLU  |
| 3   | D     | 33   | ASN  |
| 3   | D     | 36   | THR  |
| 3   | D     | 60   | CYS  |
| 3   | D     | 74   | GLU  |
| 3   | D     | 81   | THR  |
| 3   | D     | 87   | ARG  |
| 3   | D     | 111  | LYS  |
| 3   | D     | 133  | ILE  |
| 3   | D     | 135  | LEU  |
| 3   | D     | 142  | LEU  |
| 3   | D     | 153  | LEU  |
| 3   | D     | 156  | GLU  |
| 3   | D     | 171  | LEU  |
| 3   | D     | 172  | PRO  |
| 3   | D     | 178  | LEU  |
| 3   | D     | 248  | PRO  |
| 3   | D     | 291  | LEU  |
| 3   | D     | 297  | ILE  |
| 3   | D     | 334  | THR  |
| 3   | D     | 336  | PHE  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 338 | GLU  |
| 3   | D     | 351 | MET  |
| 3   | D     | 361 | VAL  |
| 3   | D     | 387 | LEU  |
| 3   | D     | 404 | GLU  |
| 3   | D     | 413 | ASP  |
| 3   | D     | 430 | ASP  |
| 3   | D     | 438 | ASP  |
| 3   | D     | 442 | ASN  |
| 3   | D     | 445 | ARG  |
| 3   | D     | 450 | TYR  |
| 3   | D     | 451 | ASP  |
| 3   | D     | 473 | LEU  |
| 3   | D     | 502 | PHE  |
| 3   | D     | 511 | TRP  |
| 3   | D     | 535 | PHE  |
| 3   | D     | 537 | THR  |
| 3   | D     | 542 | ASP  |
| 3   | D     | 546 | ARG  |
| 3   | D     | 564 | GLU  |
| 3   | D     | 565 | ILE  |
| 3   | D     | 569 | ASN  |
| 3   | D     | 594 | PRO  |
| 3   | D     | 602 | SER  |
| 3   | D     | 604 | THR  |
| 3   | D     | 605 | ASP  |
| 3   | D     | 614 | PHE  |
| 3   | D     | 617 | ASN  |
| 3   | D     | 618 | LEU  |
| 3   | D     | 624 | ASP  |
| 3   | D     | 653 | PHE  |
| 3   | D     | 685 | ASP  |
| 3   | D     | 724 | GLN  |
| 3   | D     | 745 | MET  |
| 3   | D     | 754 | PHE  |
| 3   | D     | 756 | GLN  |
| 3   | D     | 776 | GLU  |
| 3   | D     | 782 | SER  |
| 3   | D     | 784 | ASP  |
| 3   | D     | 792 | ILE  |
| 3   | D     | 797 | LYS  |
| 3   | D     | 800 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 828  | LYS  |
| 3   | D     | 829  | VAL  |
| 3   | D     | 847  | ASP  |
| 3   | D     | 851  | LEU  |
| 3   | D     | 907  | GLU  |
| 3   | D     | 914  | LEU  |
| 3   | D     | 936  | TYR  |
| 3   | D     | 937  | TYR  |
| 3   | D     | 952  | ASP  |
| 3   | D     | 972  | LEU  |
| 3   | D     | 991  | GLN  |
| 3   | D     | 997  | THR  |
| 3   | D     | 1018 | ASN  |
| 3   | D     | 1029 | ARG  |
| 3   | D     | 1067 | VAL  |
| 3   | D     | 1083 | ASP  |
| 3   | D     | 1084 | THR  |
| 3   | D     | 1095 | THR  |
| 3   | D     | 1104 | GLU  |
| 3   | D     | 1124 | GLN  |
| 3   | D     | 1130 | ARG  |
| 3   | D     | 1139 | ASP  |
| 3   | D     | 1167 | SER  |
| 3   | D     | 1190 | SER  |
| 3   | D     | 1211 | MET  |
| 3   | D     | 1213 | ARG  |
| 3   | D     | 1217 | ILE  |
| 3   | D     | 1239 | ARG  |
| 3   | D     | 1252 | ILE  |
| 3   | D     | 1269 | LYS  |
| 3   | D     | 1285 | GLU  |
| 3   | D     | 1299 | PHE  |
| 3   | D     | 1307 | LYS  |
| 3   | D     | 1337 | GLU  |
| 3   | D     | 1342 | GLU  |
| 3   | D     | 1346 | ARG  |
| 3   | D     | 1350 | GLU  |
| 3   | D     | 1396 | GLU  |
| 3   | D     | 1398 | TRP  |
| 3   | D     | 1401 | GLU  |
| 3   | D     | 1405 | GLU  |
| 3   | D     | 1434 | TRP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1442 | ASN  |
| 3   | D     | 1458 | GLU  |
| 3   | D     | 1472 | ILE  |
| 3   | D     | 1479 | ASP  |
| 3   | D     | 1483 | PHE  |
| 3   | D     | 1495 | ILE  |
| 3   | D     | 1499 | ARG  |
| 4   | E     | 23   | VAL  |
| 4   | E     | 37   | ASN  |
| 4   | E     | 55   | PHE  |
| 4   | E     | 57   | ASP  |
| 4   | E     | 83   | ASP  |
| 4   | E     | 85   | LEU  |
| 4   | E     | 93   | TYR  |
| 5   | F     | 110  | MET  |
| 5   | F     | 118  | GLU  |
| 5   | F     | 150  | THR  |
| 5   | F     | 174  | LEU  |
| 5   | F     | 218  | GLN  |
| 5   | F     | 228  | GLU  |
| 5   | F     | 245  | GLN  |
| 5   | F     | 257  | THR  |
| 5   | F     | 287  | THR  |
| 5   | F     | 291  | ILE  |
| 5   | F     | 302  | LYS  |
| 5   | F     | 308  | LEU  |
| 5   | F     | 312  | GLN  |
| 5   | F     | 313  | GLU  |
| 5   | F     | 314  | PRO  |
| 5   | F     | 329  | TYR  |
| 5   | F     | 335  | ASP  |
| 5   | F     | 336  | GLU  |
| 5   | F     | 343  | ASP  |
| 5   | F     | 353  | GLU  |
| 5   | F     | 360  | LYS  |
| 5   | F     | 377  | ASP  |
| 5   | F     | 379  | ARG  |
| 5   | F     | 398  | ARG  |
| 5   | F     | 405  | LEU  |
| 5   | F     | 409  | LYS  |
| 5   | F     | 410  | TYR  |
| 5   | F     | 411  | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 418 | LEU  |
| 5   | F     | 420 | ASP  |
| 1   | K     | 3   | ASP  |
| 1   | K     | 9   | PRO  |
| 1   | K     | 13  | VAL  |
| 1   | K     | 64  | GLU  |
| 1   | K     | 74  | ASP  |
| 1   | K     | 94  | LEU  |
| 1   | K     | 100 | LEU  |
| 1   | K     | 124 | ASN  |
| 1   | K     | 176 | ARG  |
| 1   | K     | 182 | GLU  |
| 1   | K     | 183 | ASP  |
| 1   | K     | 191 | ASP  |
| 1   | L     | 9   | PRO  |
| 1   | L     | 23  | PHE  |
| 1   | L     | 28  | LEU  |
| 1   | L     | 40  | LEU  |
| 1   | L     | 68  | ILE  |
| 1   | L     | 82  | LEU  |
| 1   | L     | 113 | ASP  |
| 1   | L     | 114 | PHE  |
| 1   | L     | 119 | ASP  |
| 1   | L     | 140 | MET  |
| 1   | L     | 143 | ARG  |
| 1   | L     | 145 | ASP  |
| 1   | L     | 183 | ASP  |
| 1   | L     | 193 | ASP  |
| 2   | M     | 1   | MET  |
| 2   | M     | 13  | ILE  |
| 2   | M     | 15  | LEU  |
| 2   | M     | 26  | TYR  |
| 2   | M     | 41  | ASN  |
| 2   | M     | 42  | VAL  |
| 2   | M     | 71  | TYR  |
| 2   | M     | 72  | ARG  |
| 2   | M     | 73  | LEU  |
| 2   | M     | 81  | ASP  |
| 2   | M     | 104 | ASP  |
| 2   | M     | 107 | LEU  |
| 2   | M     | 113 | VAL  |
| 2   | M     | 117 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 133 | ASP  |
| 2   | M     | 158 | TYR  |
| 2   | M     | 179 | ASN  |
| 2   | M     | 184 | MET  |
| 2   | M     | 216 | GLU  |
| 2   | M     | 226 | VAL  |
| 2   | M     | 227 | PHE  |
| 2   | M     | 230 | ARG  |
| 2   | M     | 233 | GLU  |
| 2   | M     | 239 | PHE  |
| 2   | M     | 251 | ASP  |
| 2   | M     | 269 | LEU  |
| 2   | M     | 285 | LEU  |
| 2   | M     | 289 | THR  |
| 2   | M     | 290 | LEU  |
| 2   | M     | 320 | HIS  |
| 2   | M     | 344 | PHE  |
| 2   | M     | 359 | MET  |
| 2   | M     | 361 | MET  |
| 2   | M     | 367 | LEU  |
| 2   | M     | 371 | LYS  |
| 2   | M     | 372 | LEU  |
| 2   | M     | 403 | SER  |
| 2   | M     | 429 | ASP  |
| 2   | M     | 441 | VAL  |
| 2   | M     | 463 | GLU  |
| 2   | M     | 507 | ARG  |
| 2   | M     | 516 | ARG  |
| 2   | M     | 535 | SER  |
| 2   | M     | 562 | SER  |
| 2   | M     | 566 | THR  |
| 2   | M     | 579 | VAL  |
| 2   | M     | 584 | GLU  |
| 2   | M     | 600 | ASP  |
| 2   | M     | 607 | ASP  |
| 2   | M     | 610 | ARG  |
| 2   | M     | 616 | GLU  |
| 2   | M     | 628 | PHE  |
| 2   | M     | 630 | ARG  |
| 2   | M     | 632 | ASN  |
| 2   | M     | 650 | ARG  |
| 2   | M     | 653 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 657  | ASP  |
| 2   | M     | 672  | VAL  |
| 2   | M     | 676  | ILE  |
| 2   | M     | 699  | PHE  |
| 2   | M     | 720  | GLU  |
| 2   | M     | 737  | LEU  |
| 2   | M     | 739  | GLU  |
| 2   | M     | 744  | ARG  |
| 2   | M     | 761  | PHE  |
| 2   | M     | 787  | ASP  |
| 2   | M     | 808  | ARG  |
| 2   | M     | 858  | MET  |
| 2   | M     | 861  | LEU  |
| 2   | M     | 876  | VAL  |
| 2   | M     | 879  | ARG  |
| 2   | M     | 881  | ASN  |
| 2   | M     | 916  | GLU  |
| 2   | M     | 953  | VAL  |
| 2   | M     | 958  | THR  |
| 2   | M     | 971  | LYS  |
| 2   | M     | 975  | TYR  |
| 2   | M     | 976  | ASP  |
| 2   | M     | 988  | VAL  |
| 2   | M     | 1003 | ASP  |
| 2   | M     | 1058 | ASP  |
| 2   | M     | 1059 | ASP  |
| 3   | N     | 16   | GLU  |
| 3   | N     | 33   | ASN  |
| 3   | N     | 36   | THR  |
| 3   | N     | 81   | THR  |
| 3   | N     | 87   | ARG  |
| 3   | N     | 111  | LYS  |
| 3   | N     | 112  | ILE  |
| 3   | N     | 119  | SER  |
| 3   | N     | 125  | GLN  |
| 3   | N     | 131  | LYS  |
| 3   | N     | 133  | ILE  |
| 3   | N     | 135  | LEU  |
| 3   | N     | 149  | LYS  |
| 3   | N     | 167  | GLU  |
| 3   | N     | 206  | ARG  |
| 3   | N     | 213  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 224 | ARG  |
| 3   | N     | 226 | PRO  |
| 3   | N     | 315 | ARG  |
| 3   | N     | 337 | LEU  |
| 3   | N     | 338 | GLU  |
| 3   | N     | 350 | HIS  |
| 3   | N     | 351 | MET  |
| 3   | N     | 387 | LEU  |
| 3   | N     | 392 | SER  |
| 3   | N     | 404 | GLU  |
| 3   | N     | 430 | ASP  |
| 3   | N     | 432 | TYR  |
| 3   | N     | 434 | ARG  |
| 3   | N     | 441 | ARG  |
| 3   | N     | 445 | ARG  |
| 3   | N     | 450 | TYR  |
| 3   | N     | 451 | ASP  |
| 3   | N     | 456 | MET  |
| 3   | N     | 470 | LEU  |
| 3   | N     | 481 | MET  |
| 3   | N     | 485 | SER  |
| 3   | N     | 500 | ARG  |
| 3   | N     | 502 | PHE  |
| 3   | N     | 511 | TRP  |
| 3   | N     | 535 | PHE  |
| 3   | N     | 564 | GLU  |
| 3   | N     | 565 | ILE  |
| 3   | N     | 566 | ILE  |
| 3   | N     | 602 | SER  |
| 3   | N     | 605 | ASP  |
| 3   | N     | 614 | PHE  |
| 3   | N     | 617 | ASN  |
| 3   | N     | 618 | LEU  |
| 3   | N     | 624 | ASP  |
| 3   | N     | 653 | PHE  |
| 3   | N     | 669 | ASN  |
| 3   | N     | 692 | GLU  |
| 3   | N     | 724 | GLN  |
| 3   | N     | 725 | SER  |
| 3   | N     | 734 | GLU  |
| 3   | N     | 745 | MET  |
| 3   | N     | 754 | PHE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 762  | GLN  |
| 3   | N     | 769  | LEU  |
| 3   | N     | 778  | LEU  |
| 3   | N     | 784  | ASP  |
| 3   | N     | 798  | GLU  |
| 3   | N     | 799  | LYS  |
| 3   | N     | 800  | LYS  |
| 3   | N     | 809  | PRO  |
| 3   | N     | 828  | LYS  |
| 3   | N     | 829  | VAL  |
| 3   | N     | 832  | ARG  |
| 3   | N     | 847  | ASP  |
| 3   | N     | 867  | ARG  |
| 3   | N     | 875  | THR  |
| 3   | N     | 907  | GLU  |
| 3   | N     | 921  | ARG  |
| 3   | N     | 936  | TYR  |
| 3   | N     | 941  | PHE  |
| 3   | N     | 947  | ILE  |
| 3   | N     | 965  | GLU  |
| 3   | N     | 972  | LEU  |
| 3   | N     | 985  | ASP  |
| 3   | N     | 990  | ASP  |
| 3   | N     | 991  | GLN  |
| 3   | N     | 999  | THR  |
| 3   | N     | 1021 | TYR  |
| 3   | N     | 1067 | VAL  |
| 3   | N     | 1084 | THR  |
| 3   | N     | 1087 | ARG  |
| 3   | N     | 1095 | THR  |
| 3   | N     | 1130 | ARG  |
| 3   | N     | 1139 | ASP  |
| 3   | N     | 1167 | SER  |
| 3   | N     | 1188 | VAL  |
| 3   | N     | 1201 | CYS  |
| 3   | N     | 1213 | ARG  |
| 3   | N     | 1215 | VAL  |
| 3   | N     | 1217 | ILE  |
| 3   | N     | 1239 | ARG  |
| 3   | N     | 1251 | ASP  |
| 3   | N     | 1263 | PHE  |
| 3   | N     | 1267 | ARG  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1285 | GLU  |
| 3   | N     | 1299 | PHE  |
| 3   | N     | 1307 | LYS  |
| 3   | N     | 1308 | GLU  |
| 3   | N     | 1337 | GLU  |
| 3   | N     | 1342 | GLU  |
| 3   | N     | 1346 | ARG  |
| 3   | N     | 1387 | SER  |
| 3   | N     | 1401 | GLU  |
| 3   | N     | 1405 | GLU  |
| 3   | N     | 1430 | SER  |
| 3   | N     | 1434 | TRP  |
| 3   | N     | 1439 | SER  |
| 3   | N     | 1441 | GLN  |
| 3   | N     | 1442 | ASN  |
| 3   | N     | 1449 | GLU  |
| 3   | N     | 1460 | ILE  |
| 3   | N     | 1464 | GLU  |
| 3   | N     | 1472 | ILE  |
| 3   | N     | 1479 | ASP  |
| 3   | N     | 1485 | GLN  |
| 3   | N     | 1495 | ILE  |
| 3   | N     | 1499 | ARG  |
| 4   | O     | 23   | VAL  |
| 4   | O     | 37   | ASN  |
| 4   | O     | 40   | LEU  |
| 4   | O     | 57   | ASP  |
| 4   | O     | 83   | ASP  |
| 4   | O     | 85   | LEU  |
| 4   | O     | 86   | GLN  |
| 4   | O     | 88   | GLU  |
| 4   | O     | 93   | TYR  |
| 5   | P     | 94   | LEU  |
| 5   | P     | 107  | GLU  |
| 5   | P     | 118  | GLU  |
| 5   | P     | 138  | SER  |
| 5   | P     | 143  | HIS  |
| 5   | P     | 156  | VAL  |
| 5   | P     | 163  | LEU  |
| 5   | P     | 212  | LEU  |
| 5   | P     | 233  | PHE  |
| 5   | P     | 245  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | P     | 257 | THR  |
| 5   | P     | 264 | MET  |
| 5   | P     | 287 | THR  |
| 5   | P     | 291 | ILE  |
| 5   | P     | 302 | LYS  |
| 5   | P     | 306 | GLU  |
| 5   | P     | 308 | LEU  |
| 5   | P     | 313 | GLU  |
| 5   | P     | 314 | PRO  |
| 5   | P     | 327 | SER  |
| 5   | P     | 328 | PHE  |
| 5   | P     | 329 | TYR  |
| 5   | P     | 331 | ASP  |
| 5   | P     | 334 | PRO  |
| 5   | P     | 336 | GLU  |
| 5   | P     | 353 | GLU  |
| 5   | P     | 355 | GLU  |
| 5   | P     | 367 | MET  |
| 5   | P     | 373 | LYS  |
| 5   | P     | 379 | ARG  |
| 5   | P     | 382 | THR  |
| 5   | P     | 409 | LYS  |
| 5   | P     | 410 | TYR  |
| 5   | P     | 411 | HIS  |
| 5   | P     | 414 | ARG  |
| 5   | P     | 418 | LEU  |
| 5   | P     | 420 | ASP  |
| 5   | P     | 422 | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 16  | GLN  |
| 1   | A     | 81  | ASN  |
| 1   | A     | 91  | ASN  |
| 1   | A     | 95  | GLN  |
| 1   | A     | 128 | HIS  |
| 1   | A     | 163 | ASN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 188 | GLN  |
| 1   | A     | 212 | ASN  |
| 1   | A     | 213 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 221  | HIS  |
| 1   | B     | 91   | ASN  |
| 1   | B     | 95   | GLN  |
| 1   | B     | 128  | HIS  |
| 1   | B     | 139  | ASN  |
| 2   | C     | 31   | GLN  |
| 2   | C     | 91   | GLN  |
| 2   | C     | 99   | GLN  |
| 2   | C     | 117  | HIS  |
| 2   | C     | 130  | ASN  |
| 2   | C     | 141  | HIS  |
| 2   | C     | 179  | ASN  |
| 2   | C     | 204  | GLN  |
| 2   | C     | 374  | ASN  |
| 2   | C     | 390  | GLN  |
| 2   | C     | 393  | GLN  |
| 2   | C     | 575  | GLN  |
| 2   | C     | 683  | ASN  |
| 2   | C     | 704  | HIS  |
| 2   | C     | 829  | GLN  |
| 2   | C     | 881  | ASN  |
| 2   | C     | 889  | HIS  |
| 2   | C     | 969  | GLN  |
| 2   | C     | 991  | GLN  |
| 2   | C     | 1006 | HIS  |
| 2   | C     | 1018 | GLN  |
| 2   | C     | 1100 | GLN  |
| 2   | C     | 1107 | ASN  |
| 3   | D     | 316  | GLN  |
| 3   | D     | 442  | ASN  |
| 3   | D     | 549  | ASN  |
| 3   | D     | 552  | ASN  |
| 3   | D     | 569  | ASN  |
| 3   | D     | 680  | GLN  |
| 3   | D     | 696  | HIS  |
| 3   | D     | 703  | ASN  |
| 3   | D     | 727  | GLN  |
| 3   | D     | 729  | HIS  |
| 3   | D     | 744  | GLN  |
| 3   | D     | 748  | HIS  |
| 3   | D     | 824  | ASN  |
| 3   | D     | 906  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 962  | GLN  |
| 3   | D     | 973  | GLN  |
| 3   | D     | 994  | GLN  |
| 3   | D     | 1010 | ASN  |
| 3   | D     | 1014 | ASN  |
| 3   | D     | 1034 | GLN  |
| 3   | D     | 1103 | HIS  |
| 3   | D     | 1124 | GLN  |
| 3   | D     | 1172 | HIS  |
| 3   | D     | 1359 | GLN  |
| 3   | D     | 1442 | ASN  |
| 3   | D     | 1489 | GLN  |
| 4   | E     | 28   | GLN  |
| 4   | E     | 86   | GLN  |
| 5   | F     | 83   | GLN  |
| 5   | F     | 170  | HIS  |
| 5   | F     | 214  | GLN  |
| 5   | F     | 217  | ASN  |
| 5   | F     | 245  | GLN  |
| 5   | F     | 263  | HIS  |
| 5   | F     | 269  | ASN  |
| 5   | F     | 347  | GLN  |
| 5   | F     | 399  | GLN  |
| 5   | F     | 402  | ASN  |
| 5   | F     | 411  | HIS  |
| 1   | K     | 38   | ASN  |
| 1   | K     | 81   | ASN  |
| 1   | K     | 128  | HIS  |
| 1   | K     | 163  | ASN  |
| 1   | K     | 188  | GLN  |
| 1   | K     | 212  | ASN  |
| 1   | L     | 38   | ASN  |
| 1   | L     | 91   | ASN  |
| 1   | L     | 95   | GLN  |
| 1   | L     | 128  | HIS  |
| 1   | L     | 156  | HIS  |
| 1   | L     | 188  | GLN  |
| 1   | L     | 212  | ASN  |
| 2   | M     | 41   | ASN  |
| 2   | M     | 91   | GLN  |
| 2   | M     | 179  | ASN  |
| 2   | M     | 330  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 374  | ASN  |
| 2   | M     | 390  | GLN  |
| 2   | M     | 434  | HIS  |
| 2   | M     | 567  | GLN  |
| 2   | M     | 575  | GLN  |
| 2   | M     | 632  | ASN  |
| 2   | M     | 633  | GLN  |
| 2   | M     | 860  | HIS  |
| 2   | M     | 881  | ASN  |
| 2   | M     | 899  | GLN  |
| 2   | M     | 969  | GLN  |
| 2   | M     | 1047 | HIS  |
| 2   | M     | 1050 | GLN  |
| 2   | M     | 1100 | GLN  |
| 2   | M     | 1107 | ASN  |
| 3   | N     | 316  | GLN  |
| 3   | N     | 552  | ASN  |
| 3   | N     | 569  | ASN  |
| 3   | N     | 617  | ASN  |
| 3   | N     | 703  | ASN  |
| 3   | N     | 714  | GLN  |
| 3   | N     | 729  | HIS  |
| 3   | N     | 744  | GLN  |
| 3   | N     | 824  | ASN  |
| 3   | N     | 962  | GLN  |
| 3   | N     | 973  | GLN  |
| 3   | N     | 994  | GLN  |
| 3   | N     | 1103 | HIS  |
| 3   | N     | 1323 | GLN  |
| 3   | N     | 1442 | ASN  |
| 3   | N     | 1489 | GLN  |
| 4   | O     | 28   | GLN  |
| 4   | O     | 29   | GLN  |
| 4   | O     | 33   | HIS  |
| 4   | O     | 86   | GLN  |
| 5   | P     | 170  | HIS  |
| 5   | P     | 186  | HIS  |
| 5   | P     | 214  | GLN  |
| 5   | P     | 217  | ASN  |
| 5   | P     | 245  | GLN  |
| 5   | P     | 254  | GLN  |
| 5   | P     | 269  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | P     | 279 | GLN  |
| 5   | P     | 347 | GLN  |
| 5   | P     | 399 | GLN  |
| 5   | P     | 402 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 8   | MPD  | C     | 1121 | -    | 7,7,7        | 2.24 | 1 (14%)     | 9,10,10     | 1.11 | 0           |
| 6   | PO4  | D     | 1528 | -    | 4,4,4        | 1.63 | 0           | 6,6,6       | 0.44 | 0           |
| 6   | PO4  | A     | 316  | -    | 4,4,4        | 1.57 | 0           | 6,6,6       | 0.44 | 0           |
| 8   | MPD  | C     | 1120 | -    | 7,7,7        | 2.22 | 1 (14%)     | 9,10,10     | 1.16 | 0           |
| 10  | NE6  | N     | 1528 | -    | 29,30,30     | 3.64 | 7 (24%)     | 27,39,39    | 1.81 | 4 (14%)     |
| 10  | NE6  | D     | 1529 | -    | 29,30,30     | 3.60 | 7 (24%)     | 27,39,39    | 1.77 | 4 (14%)     |
| 8   | MPD  | M     | 1120 | -    | 7,7,7        | 2.12 | 1 (14%)     | 9,10,10     | 1.09 | 0           |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals  | Torsions    | Rings   |
|-----|------|-------|------|------|----------|-------------|---------|
| 8   | MPD  | C     | 1121 | -    | -        | 0/5/5/5     | -       |
| 10  | NE6  | N     | 1528 | -    | 1/1/9/13 | 11/26/46/46 | 0/1/1/1 |
| 10  | NE6  | D     | 1529 | -    | 1/1/9/13 | 9/26/46/46  | 0/1/1/1 |
| 8   | MPD  | C     | 1120 | -    | -        | 5/5/5/5     | -       |
| 8   | MPD  | M     | 1120 | -    | -        | 2/5/5/5     | -       |

All (17) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 10  | N     | 1528 | NE6  | C11-C12 | -14.72 | 1.35        | 1.49     |
| 10  | D     | 1529 | NE6  | C11-C12 | -14.09 | 1.35        | 1.49     |
| 10  | D     | 1529 | NE6  | O4-C4   | 10.74  | 1.38        | 1.22     |
| 10  | N     | 1528 | NE6  | O4-C4   | 10.57  | 1.38        | 1.22     |
| 8   | C     | 1121 | MPD  | O2-C2   | -5.47  | 1.30        | 1.44     |
| 8   | C     | 1120 | MPD  | O2-C2   | -5.44  | 1.30        | 1.44     |
| 8   | M     | 1120 | MPD  | O2-C2   | -5.15  | 1.31        | 1.44     |
| 10  | D     | 1529 | NE6  | C12-N12 | 3.37   | 1.39        | 1.26     |
| 10  | N     | 1528 | NE6  | C3-C4   | -3.30  | 1.39        | 1.50     |
| 10  | D     | 1529 | NE6  | C3-C4   | -3.28  | 1.39        | 1.50     |
| 10  | N     | 1528 | NE6  | C19-C20 | 3.17   | 1.37        | 1.34     |
| 10  | D     | 1529 | NE6  | C15-C16 | 3.07   | 1.53        | 1.48     |
| 10  | N     | 1528 | NE6  | C12-N12 | 2.94   | 1.37        | 1.26     |
| 10  | D     | 1529 | NE6  | C19-C20 | 2.56   | 1.36        | 1.34     |
| 10  | N     | 1528 | NE6  | C15-C16 | 2.42   | 1.52        | 1.48     |
| 10  | D     | 1529 | NE6  | O14-C13 | 2.10   | 1.38        | 1.33     |
| 10  | N     | 1528 | NE6  | C3-C15  | -2.08  | 1.49        | 1.53     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | N     | 1528 | NE6  | O14-C13-N12 | 4.67  | 114.87      | 108.77   |
| 10  | D     | 1529 | NE6  | O14-C13-N12 | 4.36  | 114.46      | 108.77   |
| 10  | D     | 1529 | NE6  | O1-C2-O2    | 4.30  | 121.05      | 116.94   |
| 10  | N     | 1528 | NE6  | O1-C2-O2    | 4.18  | 120.94      | 116.94   |
| 10  | D     | 1529 | NE6  | O4-C4-C5    | -3.84 | 114.87      | 121.50   |
| 10  | N     | 1528 | NE6  | O4-C4-C5    | -3.83 | 114.89      | 121.50   |
| 10  | D     | 1529 | NE6  | C4-C5-C6    | -2.92 | 119.10      | 121.20   |
| 10  | N     | 1528 | NE6  | C4-C5-C6    | -2.89 | 119.12      | 121.20   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 10  | N     | 1528 | NE6  | C3   |
| 10  | D     | 1529 | NE6  | C3   |

All (27) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 8   | C     | 1120 | MPD  | C1-C2-C3-C4     |
| 8   | C     | 1120 | MPD  | O2-C2-C3-C4     |
| 10  | N     | 1528 | NE6  | O1-C6-C7-C8     |
| 10  | N     | 1528 | NE6  | O1-C6-C7-C9     |
| 10  | N     | 1528 | NE6  | C8-C7-C9-C10    |
| 10  | N     | 1528 | NE6  | C3-C15-C16-C18  |
| 10  | N     | 1528 | NE6  | O15-C15-C16-C18 |
| 10  | D     | 1529 | NE6  | O15-C15-C3-C2   |
| 10  | D     | 1529 | NE6  | O1-C6-C7-C8     |
| 10  | D     | 1529 | NE6  | O1-C6-C7-C9     |
| 10  | D     | 1529 | NE6  | C9-C10-C11-C12  |
| 10  | D     | 1529 | NE6  | C3-C15-C16-C17  |
| 10  | N     | 1528 | NE6  | C16-C15-C3-C2   |
| 10  | N     | 1528 | NE6  | O15-C15-C3-C2   |
| 10  | D     | 1529 | NE6  | C16-C15-C3-C2   |
| 10  | N     | 1528 | NE6  | C3-C15-C16-C17  |
| 10  | N     | 1528 | NE6  | O15-C15-C16-C17 |
| 10  | D     | 1529 | NE6  | O15-C15-C16-C17 |
| 10  | D     | 1529 | NE6  | O15-C15-C16-C18 |
| 10  | N     | 1528 | NE6  | C5-C6-C7-C8     |
| 10  | D     | 1529 | NE6  | C5-C6-C7-C8     |
| 8   | C     | 1120 | MPD  | CM-C2-C3-C4     |
| 10  | N     | 1528 | NE6  | C6-C7-C9-C10    |
| 8   | C     | 1120 | MPD  | C2-C3-C4-C5     |
| 8   | M     | 1120 | MPD  | C2-C3-C4-C5     |
| 8   | C     | 1120 | MPD  | C2-C3-C4-O4     |
| 8   | M     | 1120 | MPD  | C2-C3-C4-O4     |

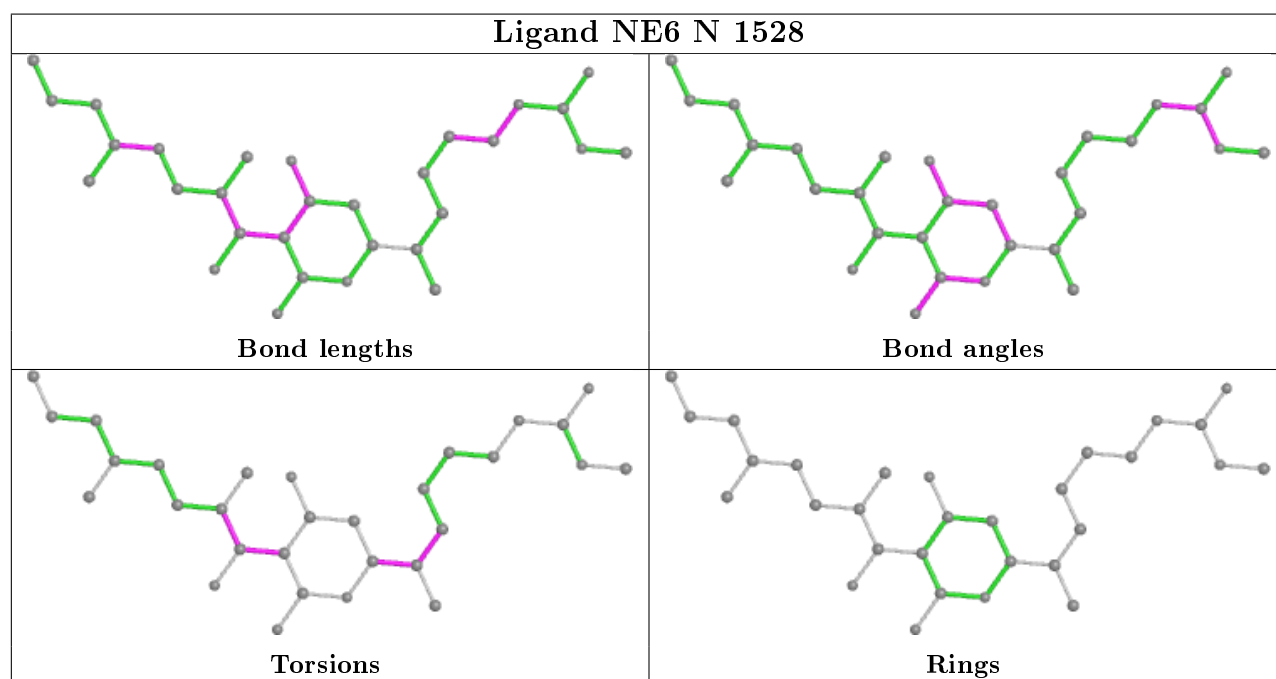
There are no ring outliers.

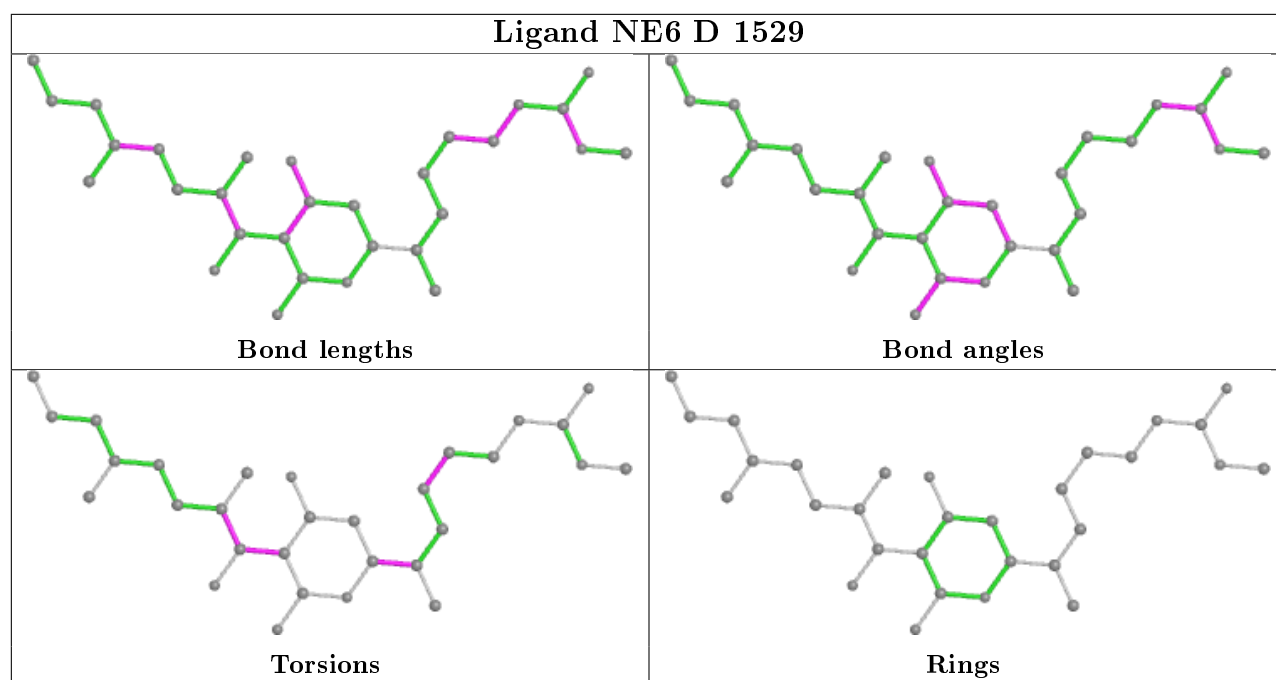
3 monomers are involved in 16 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6   | D     | 1528 | PO4  | 1       | 0            |
| 10  | N     | 1528 | NE6  | 7       | 0            |
| 10  | D     | 1529 | NE6  | 8       | 0            |



The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|--------------|-----------------------|-------|
| 1   | A     | 231/315 (73%)    | -0.66  | 0 100 100    | 43, 72, 100, 115      | 0     |
| 1   | B     | 243/315 (77%)    | -0.82  | 0 100 100    | 51, 93, 113, 117      | 0     |
| 1   | K     | 231/315 (73%)    | -0.68  | 0 100 100    | 45, 73, 105, 117      | 0     |
| 1   | L     | 243/315 (77%)    | -0.81  | 0 100 100    | 56, 89, 112, 117      | 0     |
| 2   | C     | 1119/1119 (100%) | -0.73  | 0 100 100    | 36, 77, 115, 117      | 0     |
| 2   | M     | 1119/1119 (100%) | -0.72  | 0 100 100    | 31, 79, 115, 117      | 0     |
| 3   | D     | 1504/1524 (98%)  | -0.70  | 1 (0%) 95 89 | 35, 78, 117, 117      | 0     |
| 3   | N     | 1504/1524 (98%)  | -0.68  | 3 (0%) 95 87 | 34, 75, 113, 117      | 0     |
| 4   | E     | 95/99 (95%)      | -0.81  | 0 100 100    | 51, 88, 113, 117      | 0     |
| 4   | O     | 95/99 (95%)      | -0.78  | 0 100 100    | 52, 85, 109, 116      | 0     |
| 5   | F     | 349/423 (82%)    | -0.85  | 0 100 100    | 52, 84, 110, 117      | 0     |
| 5   | P     | 349/423 (82%)    | -0.81  | 0 100 100    | 51, 85, 110, 117      | 0     |
| All | All   | 7082/7590 (93%)  | -0.72  | 4 (0%) 95 89 | 31, 79, 115, 117      | 0     |

All (4) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | N     | 243 | ALA  | 4.1  |
| 3   | N     | 242 | LEU  | 3.2  |
| 3   | N     | 328 | GLY  | 3.0  |
| 3   | D     | 329 | GLU  | 2.1  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

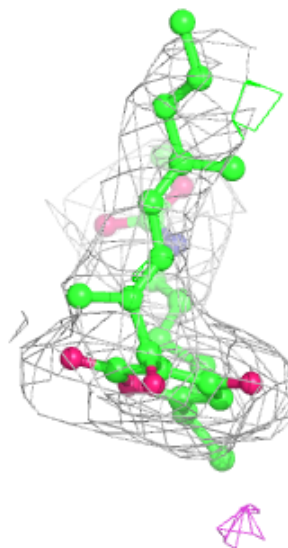
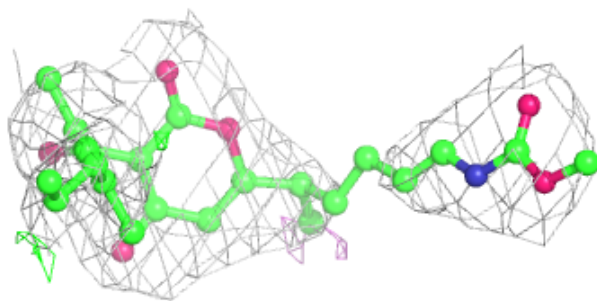
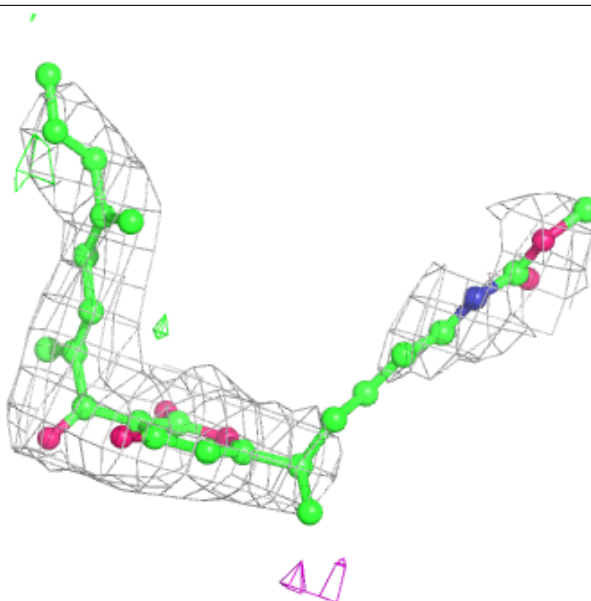
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 8   | MPD  | M     | 1120 | 8/8   | 0.92 | 0.17 | 71,79,84,85                 | 0     |
| 10  | NE6  | N     | 1528 | 30/30 | 0.94 | 0.29 | 72,84,90,91                 | 0     |
| 7   | MG   | D     | 1527 | 1/1   | 0.96 | 0.07 | 79,79,79,79                 | 0     |
| 6   | PO4  | A     | 316  | 5/5   | 0.96 | 0.18 | 71,73,77,77                 | 0     |
| 9   | ZN   | D     | 1525 | 1/1   | 0.96 | 0.17 | 91,91,91,91                 | 0     |
| 8   | MPD  | C     | 1121 | 8/8   | 0.96 | 0.15 | 70,72,73,73                 | 0     |
| 10  | NE6  | D     | 1529 | 30/30 | 0.96 | 0.22 | 52,70,81,85                 | 0     |
| 6   | PO4  | D     | 1528 | 5/5   | 0.96 | 0.14 | 86,86,86,89                 | 0     |
| 7   | MG   | N     | 1527 | 1/1   | 0.97 | 0.04 | 56,56,56,56                 | 0     |
| 7   | MG   | B     | 701  | 1/1   | 0.97 | 0.20 | 55,55,55,55                 | 0     |
| 8   | MPD  | C     | 1120 | 8/8   | 0.97 | 0.17 | 51,56,57,57                 | 0     |
| 9   | ZN   | N     | 1525 | 1/1   | 0.99 | 0.19 | 50,50,50,50                 | 0     |
| 9   | ZN   | D     | 1526 | 1/1   | 1.00 | 0.18 | 77,77,77,77                 | 0     |
| 9   | ZN   | N     | 1526 | 1/1   | 1.00 | 0.18 | 55,55,55,55                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

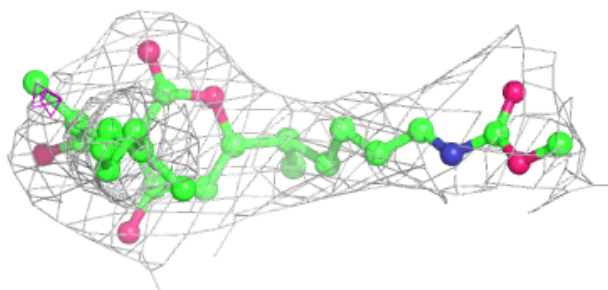
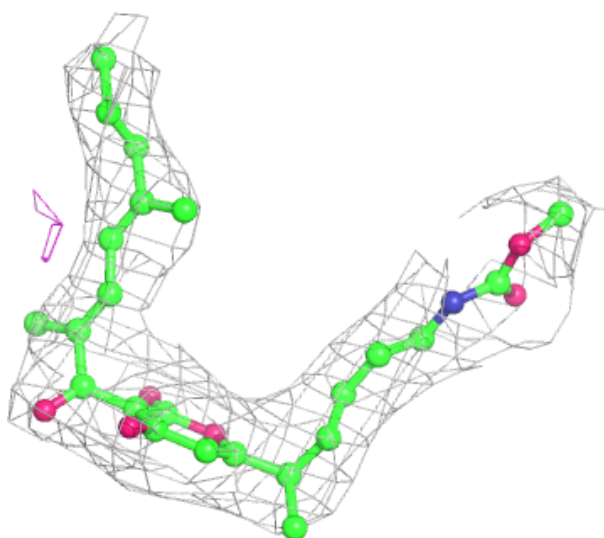
**Electron density around NE6 N 1528:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NE6 D 1529:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.