



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:37 PM GMT

PDB ID : 1G3I  
Title : CRYSTAL STRUCTURE OF THE HSLUV PROTEASE-CHAPERONE COMPLEX  
Authors : Sousa, M.C.; Trame, C.B.; Tsuruta, H.; Wilbanks, S.M.; Reddy, V.S.; McKay, D.B.  
Deposited on : 2000-10-24  
Resolution : 3.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

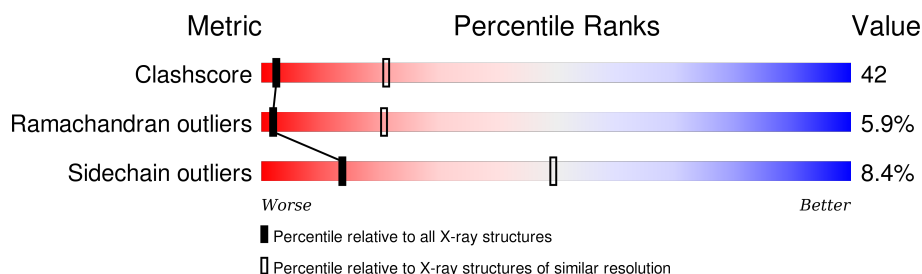
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.41 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)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 102246                      | 1032 (3.50-3.34)                                      |
| Ramachandran outliers | 100387                      | 1002 (3.50-3.34)                                      |
| Sidechain outliers    | 100360                      | 1003 (3.50-3.34)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 444    |                  |
| 1   | B     | 444    |                  |
| 1   | C     | 444    |                  |
| 1   | D     | 444    |                  |
| 1   | E     | 444    |                  |
| 1   | F     | 444    |                  |
| 1   | S     | 444    |                  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | T     | 444    |                  |
| 1   | U     | 444    |                  |
| 1   | V     | 444    |                  |
| 1   | W     | 444    |                  |
| 1   | X     | 444    |                  |
| 2   | G     | 174    |                  |
| 2   | H     | 174    |                  |
| 2   | I     | 174    |                  |
| 2   | J     | 174    |                  |
| 2   | K     | 174    |                  |
| 2   | L     | 174    |                  |
| 2   | M     | 174    |                  |
| 2   | N     | 174    |                  |
| 2   | O     | 174    |                  |
| 2   | P     | 174    |                  |
| 2   | Q     | 174    |                  |
| 2   | R     | 174    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | ATP  | E     | 454 | -         | -        | X       | -                |
| 3   | ATP  | S     | 456 | -         | -        | X       | -                |
| 3   | ATP  | U     | 458 | -         | -        | X       | -                |
| 3   | ATP  | X     | 461 | -         | -        | X       | -                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 45528 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 ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUB-UNIT HSLU.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 326      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2539  | 1588 | 454 | 487 | 10 |         |         |       |
| 1   | B     | 326      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2539  | 1588 | 454 | 487 | 10 |         |         |       |
| 1   | C     | 319      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2484  | 1554 | 446 | 474 | 10 |         |         |       |
| 1   | D     | 318      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2476  | 1548 | 445 | 473 | 10 |         |         |       |
| 1   | E     | 317      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2462  | 1540 | 443 | 469 | 10 |         |         |       |
| 1   | F     | 320      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2495  | 1560 | 450 | 475 | 10 |         |         |       |
| 1   | S     | 317      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2468  | 1543 | 444 | 471 | 10 |         |         |       |
| 1   | T     | 331      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2570  | 1602 | 461 | 497 | 10 |         |         |       |
| 1   | U     | 322      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2503  | 1562 | 449 | 482 | 10 |         |         |       |
| 1   | V     | 313      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2432  | 1519 | 436 | 467 | 10 |         |         |       |
| 1   | W     | 312      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2428  | 1516 | 437 | 465 | 10 |         |         |       |
| 1   | X     | 322      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2500  | 1562 | 446 | 482 | 10 |         |         |       |

- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

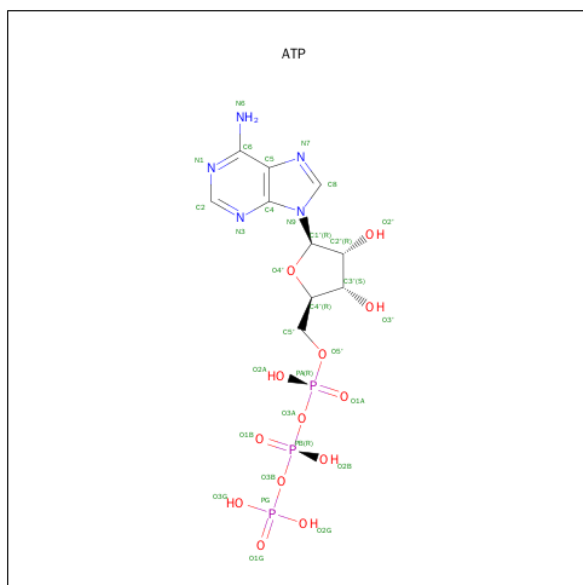
| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | G     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1280  | 803 | 227 | 246 | 4 |         |         |       |
| 2   | H     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1280  | 802 | 227 | 247 | 4 |         |         |       |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | I     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1292  | 810 | 229 | 249 | 4 |         |         |       |
| 2   | J     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1280  | 802 | 227 | 247 | 4 |         |         |       |
| 2   | K     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1280  | 802 | 227 | 247 | 4 |         |         |       |
| 2   | L     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 810 | 231 | 249 | 4 |         |         |       |
| 2   | M     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1261  | 791 | 226 | 241 | 3 |         |         |       |
| 2   | N     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1261  | 791 | 226 | 241 | 3 |         |         |       |
| 2   | O     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 789 | 225 | 240 | 3 |         |         |       |
| 2   | P     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 789 | 225 | 240 | 3 |         |         |       |
| 2   | Q     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1261  | 791 | 226 | 241 | 3 |         |         |       |
| 2   | R     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 789 | 225 | 240 | 3 |         |         |       |

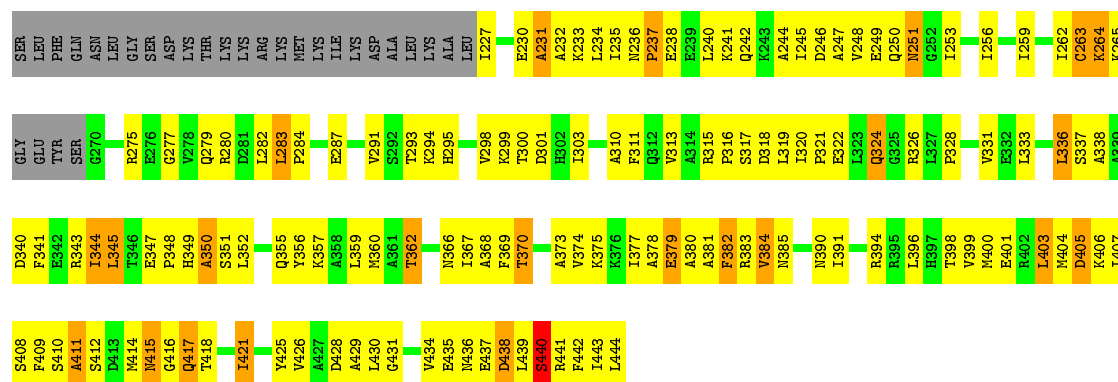
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



*Continued from previous page...*

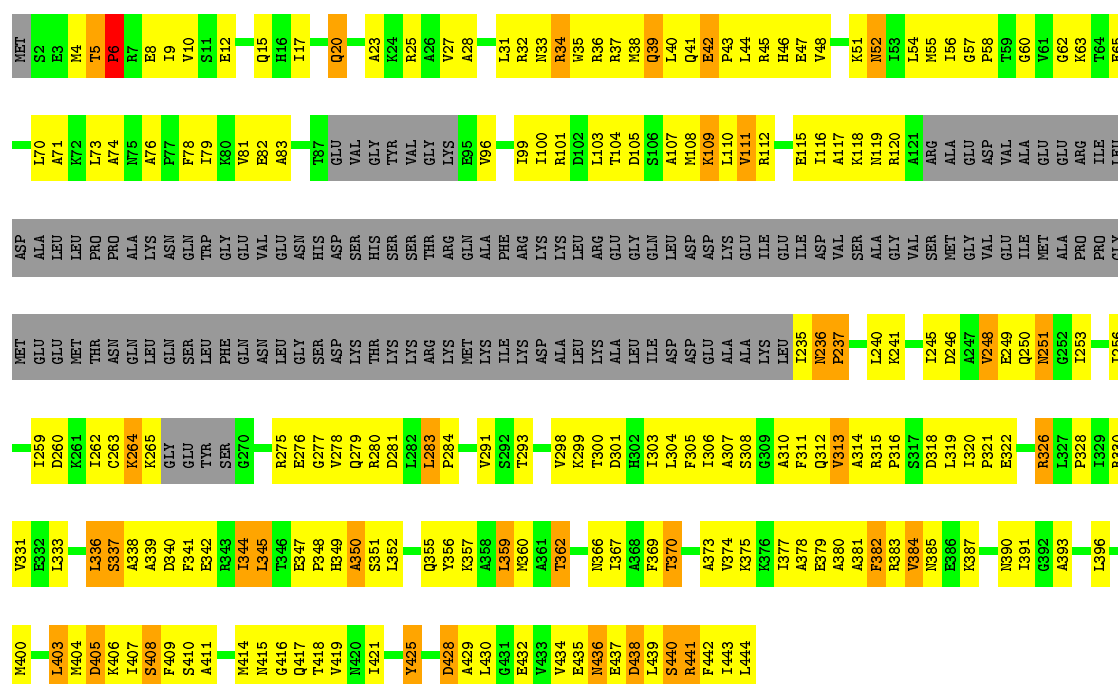
| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 3   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 3   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 3   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 3   | S     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 3   | T     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 3   | U     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 3   | V     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 3   | W     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 3   | X     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |





• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

Chain C: 26% 38% 8% 28%

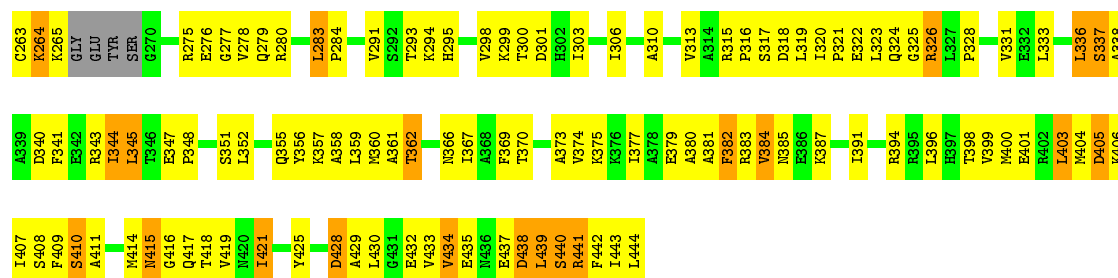


• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

Chain D: 26% 38% 7% 28%

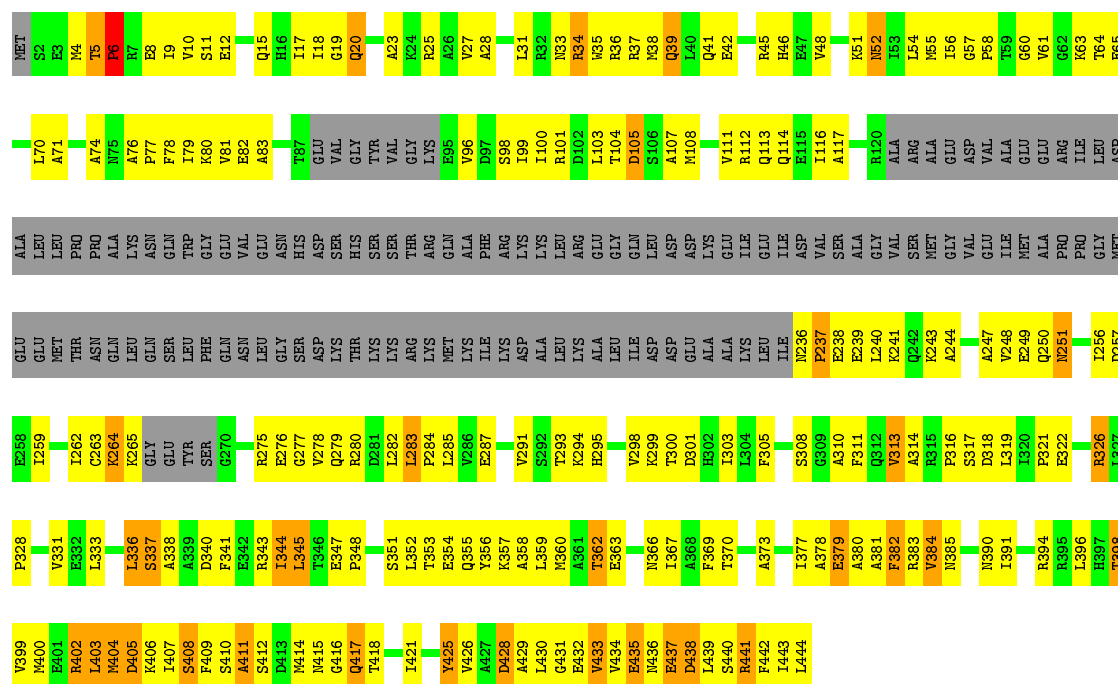






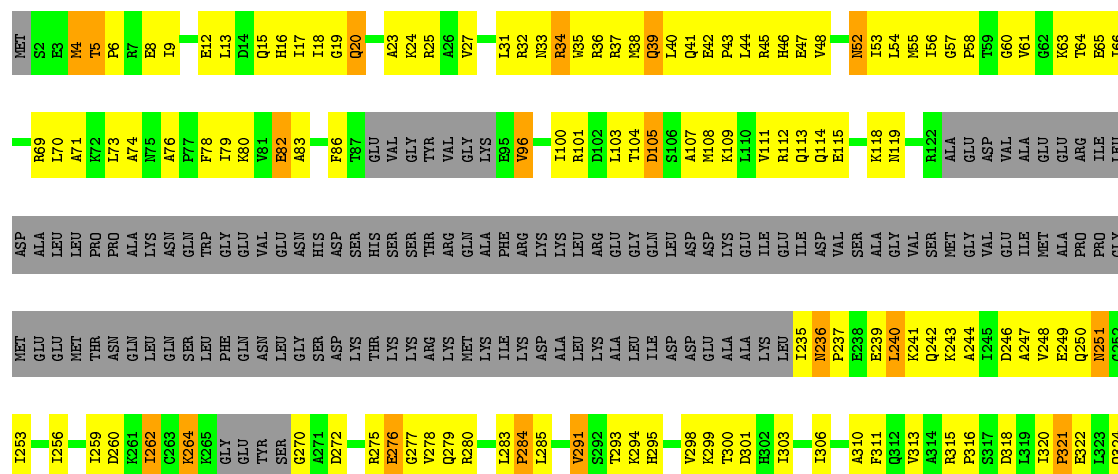
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

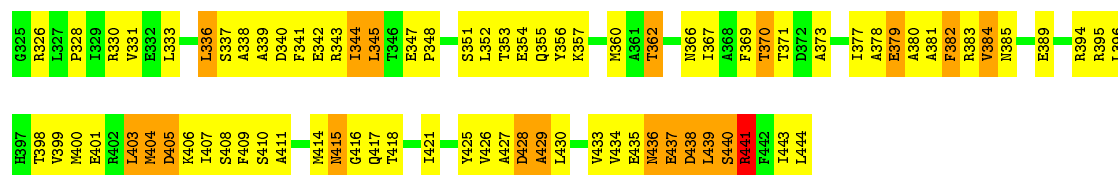
Chain E: 25% 38% 8% 29%



• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

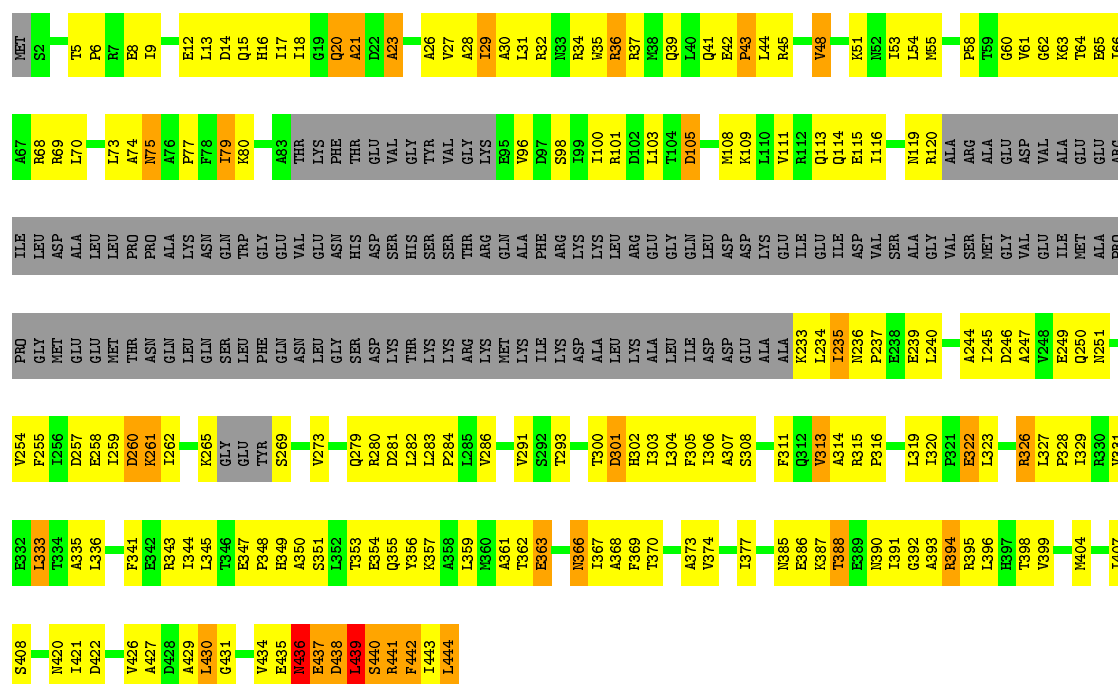
Chain F: 25% 39% 8% 28%





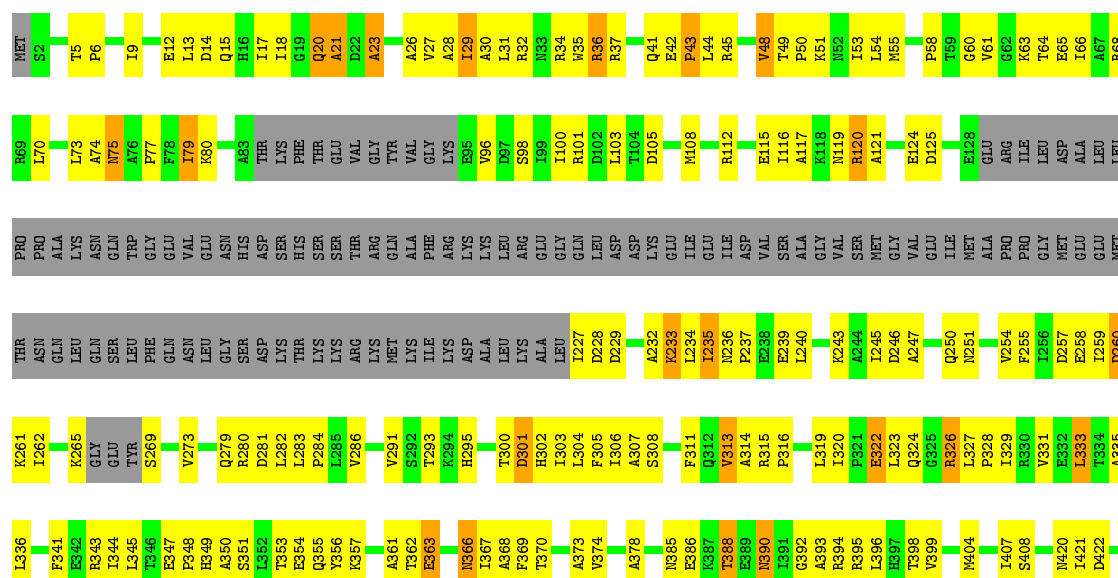
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

Chain S: 29% 36% 7% 29%

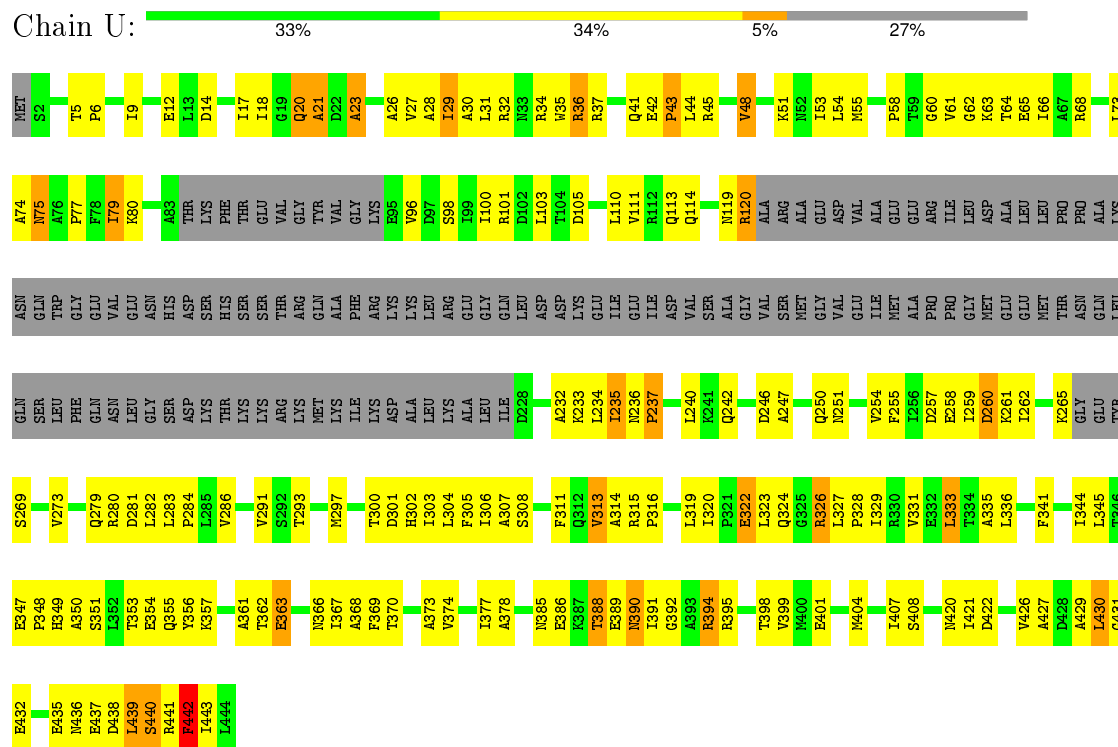


• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

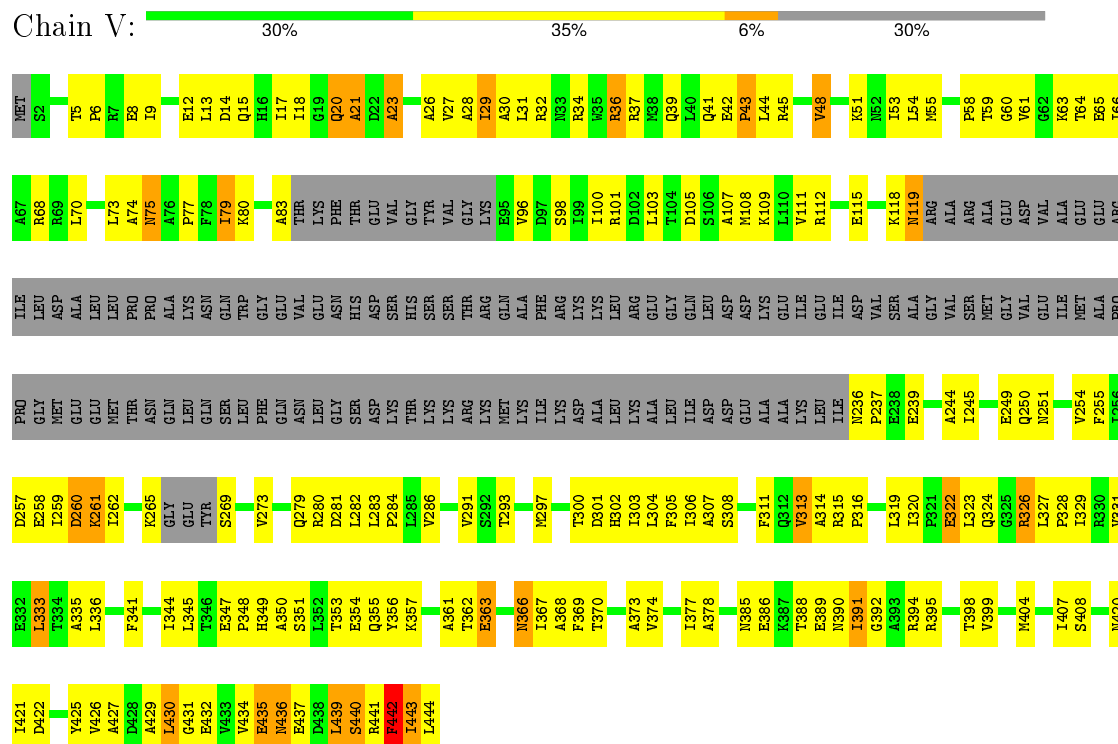
Chain T: 31% 37% 6% 25%



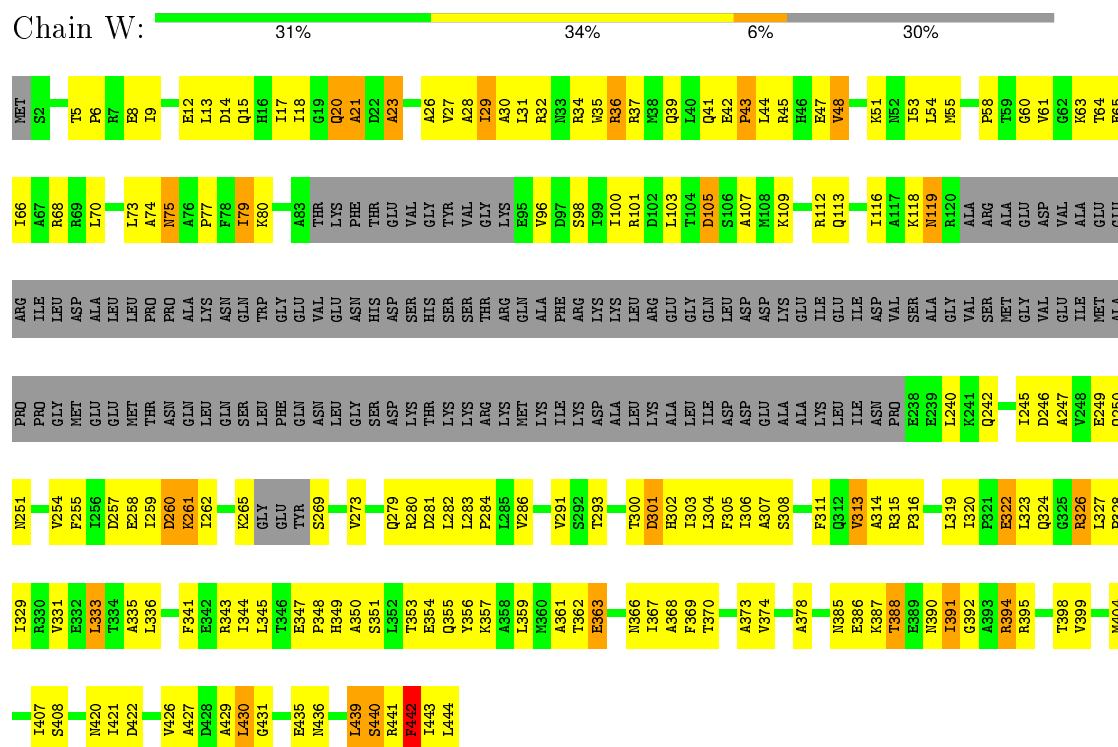
- Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU



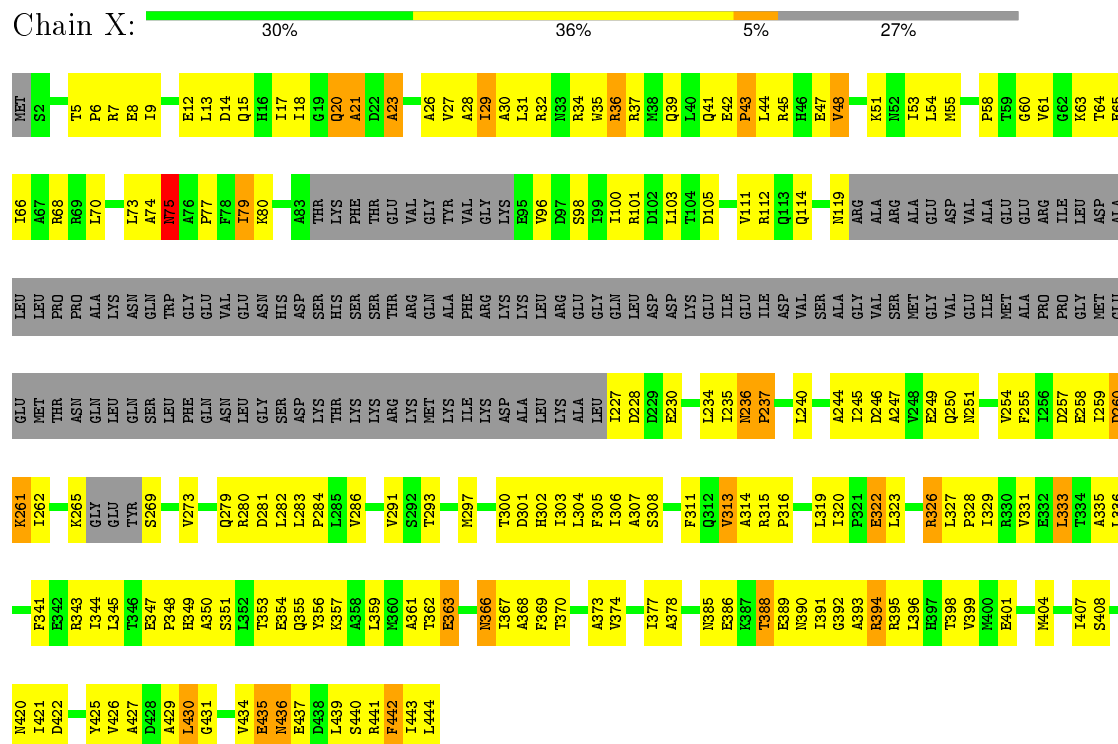
- Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU



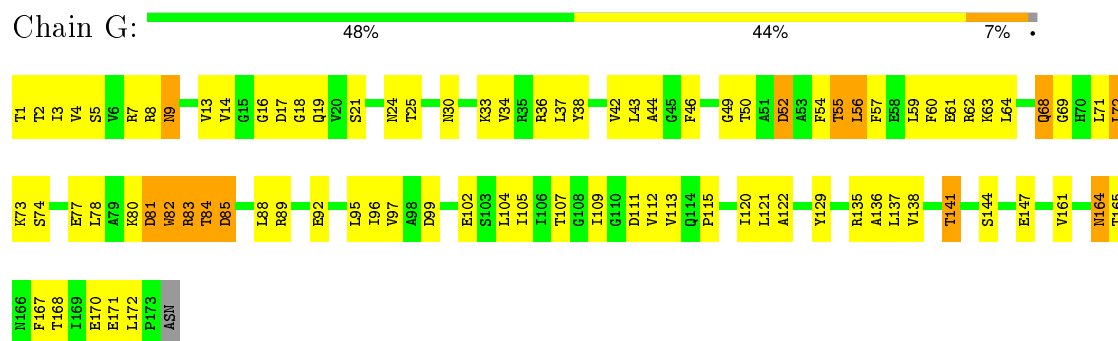
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU



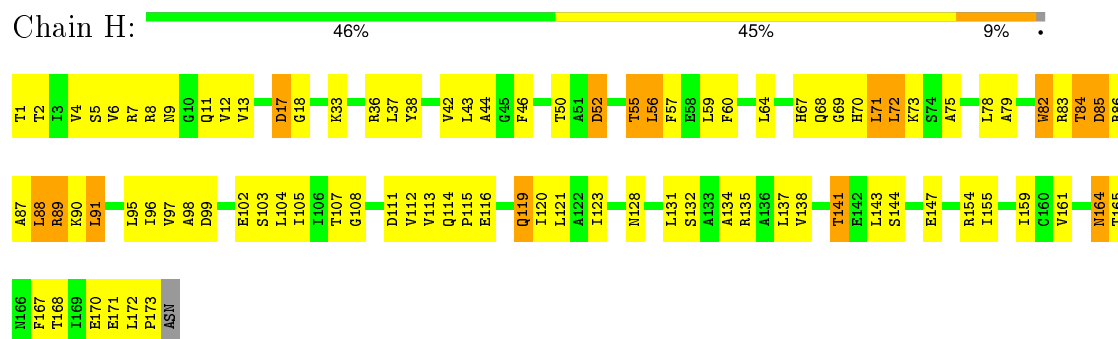
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU



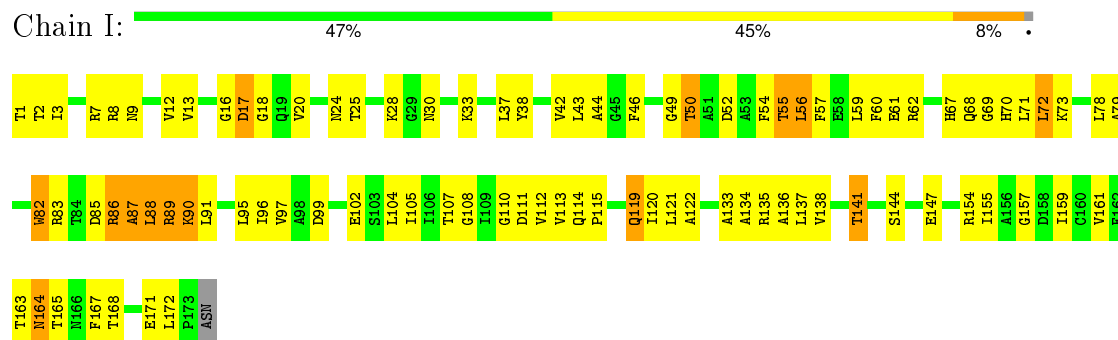
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV



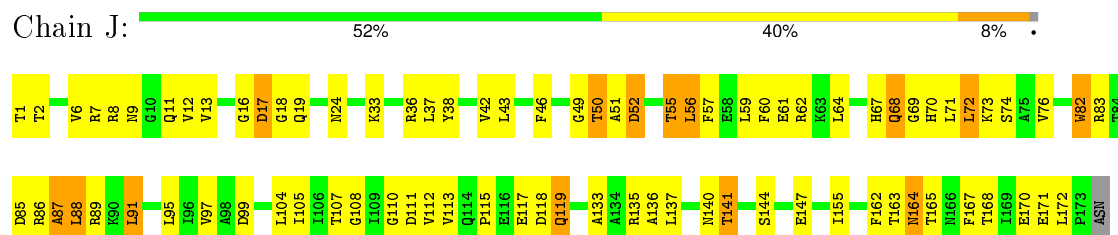
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV



- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

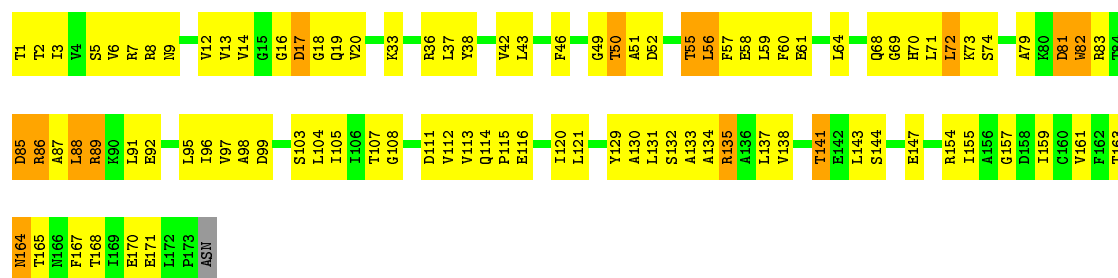


- Molecule 2: ATP-DEPENDENT PROTEASE HSLV



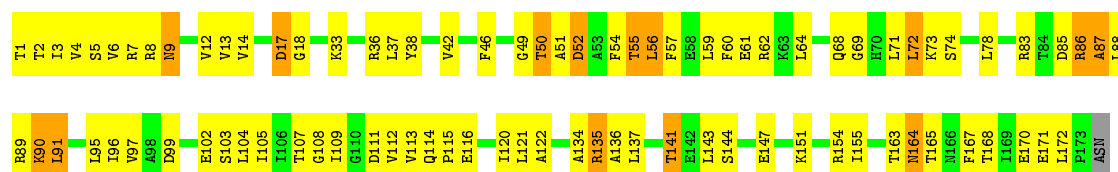
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV





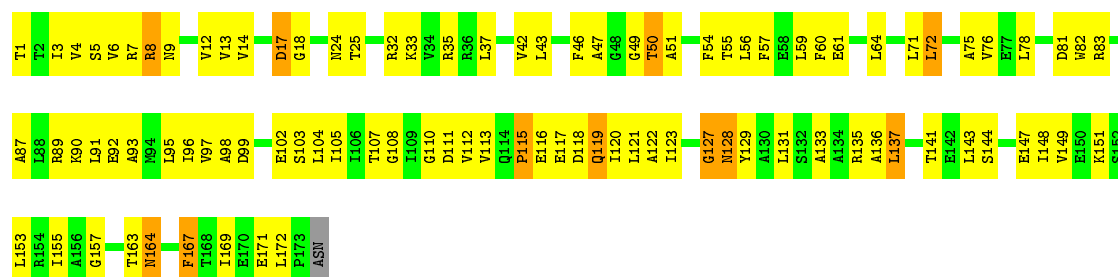
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain L: 49% 42% 8%



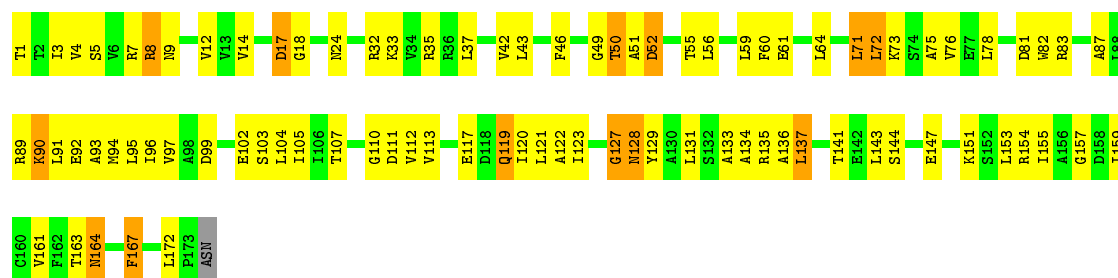
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain M: 44% 49% 6%



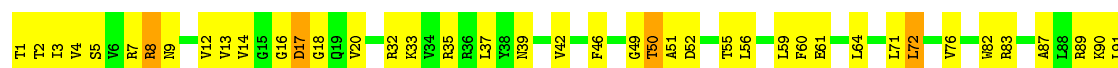
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

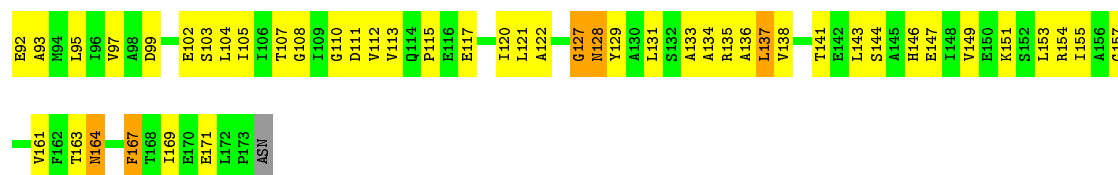
Chain N: 49% 43% 7%



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

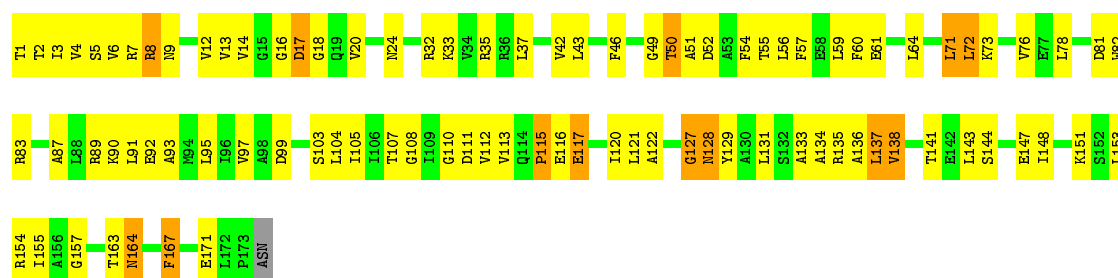
Chain O: 49% 45% 5%





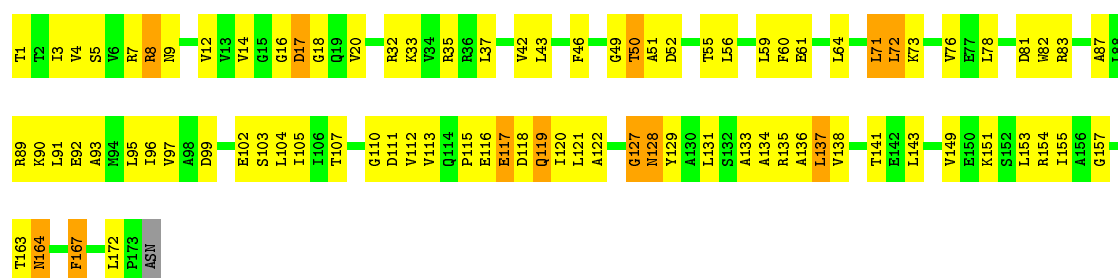
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain P: 47% 45% 7%



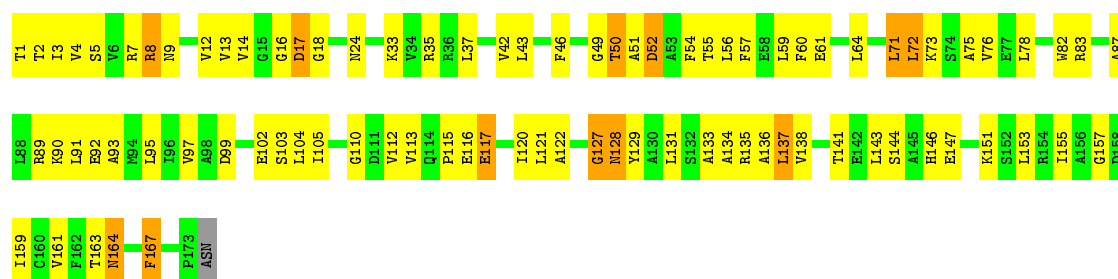
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain Q: 49% 43% 7%



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain R: 49% 43% 7%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | P 21 21 2                                       | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 209.22Å 220.58Å 241.07Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)   | 30.08 – 3.41                                    | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (30.08-3.41)                    | Depositor |
| $R_{merge}$  | 0.06  | Depositor |
| $R_{sym}$  | (Not available)                                 | Depositor |
| Refinement program                                       | CNS 1.0   | Depositor |
| R, $R_{free}$  | 0.240 , 0.284                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 45528   | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 100.0   | wwPDB-VP  |



## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 1   | A     | 0.65         | 1/2566 (0.0%)  | 0.81        | 0/3458         |
| 1   | B     | 0.62         | 0/2566         | 0.81        | 2/3458 (0.1%)  |
| 1   | C     | 0.55         | 0/2511         | 0.78        | 1/3384 (0.0%)  |
| 1   | D     | 0.64         | 1/2503 (0.0%)  | 0.82        | 1/3373 (0.0%)  |
| 1   | E     | 0.67         | 0/2489         | 0.83        | 2/3354 (0.1%)  |
| 1   | F     | 0.64         | 0/2522         | 0.79        | 0/3398         |
| 1   | S     | 0.31         | 0/2494         | 0.55        | 0/3360         |
| 1   | T     | 0.31         | 0/2596         | 0.56        | 0/3499         |
| 1   | U     | 0.30         | 0/2529         | 0.55        | 0/3408         |
| 1   | V     | 0.30         | 0/2458         | 0.55        | 0/3313         |
| 1   | W     | 0.30         | 0/2453         | 0.55        | 0/3304         |
| 1   | X     | 0.31         | 0/2526         | 0.55        | 0/3405         |
| 2   | G     | 0.55         | 0/1294         | 0.76        | 0/1753         |
| 2   | H     | 0.55         | 0/1294         | 0.78        | 0/1754         |
| 2   | I     | 0.50         | 0/1306         | 0.73        | 0/1767         |
| 2   | J     | 0.50         | 0/1294         | 0.75        | 0/1754         |
| 2   | K     | 0.52         | 0/1294         | 0.74        | 0/1754         |
| 2   | L     | 0.55         | 0/1308         | 0.77        | 0/1770         |
| 2   | M     | 0.41         | 0/1275         | 0.66        | 0/1732         |
| 2   | N     | 0.39         | 0/1275         | 0.65        | 0/1732         |
| 2   | O     | 0.35         | 0/1271         | 0.62        | 0/1727         |
| 2   | P     | 0.37         | 0/1271         | 0.63        | 0/1727         |
| 2   | Q     | 0.45         | 0/1275         | 0.65        | 0/1732         |
| 2   | R     | 0.40         | 0/1271         | 0.63        | 0/1727         |
| All | All   | 0.49         | 2/45641 (0.0%) | 0.70        | 6/61643 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 263 | CYS  | CB-SG | -8.39 | 1.68        | 1.82     |
| 1   | D     | 263 | CYS  | CB-SG | -5.66 | 1.72        | 1.81     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | E     | 283 | LEU  | CA-CB-CG | -7.04 | 99.10       | 115.30   |
| 1   | C     | 283 | LEU  | CA-CB-CG | -6.71 | 99.88       | 115.30   |
| 1   | E     | 431 | GLY  | N-CA-C   | 6.00  | 128.10      | 113.10   |
| 1   | B     | 283 | LEU  | CA-CB-CG | -5.45 | 102.76      | 115.30   |
| 1   | D     | 283 | LEU  | CA-CB-CG | -5.20 | 103.34      | 115.30   |
| 1   | B     | 37  | ARG  | N-CA-C   | -5.13 | 97.16       | 111.00   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2539  | 0        | 2606     | 238     | 0            |
| 1   | B     | 2539  | 0        | 2606     | 245     | 0            |
| 1   | C     | 2484  | 0        | 2552     | 237     | 0            |
| 1   | D     | 2476  | 0        | 2541     | 237     | 0            |
| 1   | E     | 2462  | 0        | 2521     | 241     | 0            |
| 1   | F     | 2495  | 0        | 2565     | 257     | 0            |
| 1   | S     | 2468  | 0        | 2540     | 242     | 0            |
| 1   | T     | 2570  | 0        | 2628     | 223     | 0            |
| 1   | U     | 2503  | 0        | 2564     | 225     | 0            |
| 1   | V     | 2432  | 0        | 2492     | 216     | 0            |
| 1   | W     | 2428  | 0        | 2492     | 218     | 0            |
| 1   | X     | 2500  | 0        | 2562     | 237     | 1            |
| 2   | G     | 1280  | 0        | 1275     | 107     | 0            |
| 2   | H     | 1280  | 0        | 1270     | 115     | 0            |
| 2   | I     | 1292  | 0        | 1296     | 110     | 0            |
| 2   | J     | 1280  | 0        | 1270     | 101     | 0            |
| 2   | K     | 1280  | 0        | 1270     | 111     | 0            |
| 2   | L     | 1294  | 0        | 1296     | 101     | 0            |
| 2   | M     | 1261  | 0        | 1240     | 106     | 0            |
| 2   | N     | 1261  | 0        | 1240     | 104     | 0            |
| 2   | O     | 1257  | 0        | 1234     | 98      | 0            |
| 2   | P     | 1257  | 0        | 1234     | 98      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | Q     | 1261  | 0        | 1240     | 94      | 0            |
| 2   | R     | 1257  | 0        | 1234     | 93      | 0            |
| 3   | A     | 31    | 0        | 12       | 2       | 0            |
| 3   | B     | 31    | 0        | 12       | 5       | 0            |
| 3   | C     | 31    | 0        | 12       | 5       | 0            |
| 3   | D     | 31    | 0        | 12       | 4       | 0            |
| 3   | E     | 31    | 0        | 12       | 9       | 0            |
| 3   | F     | 31    | 0        | 12       | 8       | 0            |
| 3   | S     | 31    | 0        | 12       | 14      | 0            |
| 3   | T     | 31    | 0        | 12       | 3       | 0            |
| 3   | U     | 31    | 0        | 12       | 12      | 0            |
| 3   | V     | 31    | 0        | 12       | 3       | 0            |
| 3   | W     | 31    | 0        | 12       | 8       | 0            |
| 3   | X     | 31    | 0        | 12       | 9       | 0            |
| All | All   | 45528 | 0        | 45912    | 3804    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (3804) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:264:LYS:NZ   | 1:F:279:GLN:HE22 | 1.38                     | 1.21              |
| 2:Q:7:ARG:HD2    | 2:Q:119:GLN:OE1  | 1.44                     | 1.17              |
| 1:E:264:LYS:NZ   | 1:E:279:GLN:HE22 | 1.42                     | 1.15              |
| 2:N:7:ARG:HD2    | 2:N:119:GLN:HE21 | 1.09                     | 1.15              |
| 1:A:264:LYS:NZ   | 1:A:279:GLN:HE22 | 1.45                     | 1.12              |
| 2:J:91:LEU:H     | 2:J:91:LEU:HD12  | 1.06                     | 1.11              |
| 2:I:7:ARG:HD2    | 2:I:119:GLN:OE1  | 1.50                     | 1.10              |
| 1:D:264:LYS:NZ   | 1:D:279:GLN:HE22 | 1.50                     | 1.09              |
| 1:S:313:VAL:HG23 | 1:S:314:ALA:H    | 1.19                     | 1.08              |
| 1:T:313:VAL:HG23 | 1:T:314:ALA:H    | 1.17                     | 1.08              |
| 1:U:313:VAL:HG23 | 1:U:314:ALA:H    | 1.18                     | 1.07              |
| 2:N:7:ARG:CD     | 2:N:119:GLN:HE21 | 1.69                     | 1.05              |
| 2:M:7:ARG:HD2    | 2:M:119:GLN:OE1  | 1.55                     | 1.05              |
| 1:V:279:GLN:HE21 | 1:V:320:ILE:HG12 | 1.18                     | 1.04              |
| 1:X:313:VAL:HG23 | 1:X:314:ALA:H    | 1.19                     | 1.04              |
| 1:S:279:GLN:HE21 | 1:S:320:ILE:HG12 | 1.14                     | 1.04              |
| 1:W:313:VAL:HG23 | 1:W:314:ALA:H    | 1.19                     | 1.03              |
| 1:V:313:VAL:HG23 | 1:V:314:ALA:H    | 1.19                     | 1.03              |
| 1:U:279:GLN:HE21 | 1:U:320:ILE:HG12 | 1.20                     | 1.03              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:406:LYS:HD2  | 1:F:406:LYS:H    | 1.24                     | 1.03              |
| 1:S:279:GLN:NE2  | 1:S:320:ILE:H    | 1.55                     | 1.02              |
| 1:X:279:GLN:HE21 | 1:X:320:ILE:HG12 | 1.21                     | 1.01              |
| 1:V:279:GLN:NE2  | 1:V:320:ILE:H    | 1.59                     | 1.00              |
| 1:S:279:GLN:HE22 | 1:S:320:ILE:H    | 1.10                     | 1.00              |
| 1:W:65:GLU:HG2   | 3:W:460:ATP:H5'2 | 1.41                     | 1.00              |
| 1:T:279:GLN:HE21 | 1:T:320:ILE:HG12 | 1.23                     | 1.00              |
| 1:U:279:GLN:NE2  | 1:U:320:ILE:H    | 1.59                     | 0.99              |
| 1:B:406:LYS:H    | 1:B:406:LYS:HD2  | 1.25                     | 0.99              |
| 1:U:65:GLU:HG2   | 3:U:458:ATP:H5'2 | 1.42                     | 0.99              |
| 1:C:52:ASN:ND2   | 1:C:305:PHE:H    | 1.59                     | 0.99              |
| 1:C:264:LYS:NZ   | 1:C:279:GLN:HE22 | 1.61                     | 0.99              |
| 2:O:20:VAL:HG21  | 1:V:444:LEU:HD21 | 1.41                     | 0.99              |
| 1:B:264:LYS:NZ   | 1:B:279:GLN:HE22 | 1.61                     | 0.99              |
| 1:X:279:GLN:NE2  | 1:X:320:ILE:H    | 1.61                     | 0.98              |
| 1:C:79:ILE:HG22  | 1:C:103:LEU:HD13 | 1.44                     | 0.98              |
| 1:A:406:LYS:H    | 1:A:406:LYS:HD2  | 1.24                     | 0.98              |
| 1:D:406:LYS:H    | 1:D:406:LYS:HD2  | 1.28                     | 0.98              |
| 1:W:279:GLN:NE2  | 1:W:320:ILE:H    | 1.61                     | 0.98              |
| 1:T:279:GLN:NE2  | 1:T:320:ILE:H    | 1.61                     | 0.98              |
| 2:M:115:PRO:CB   | 2:M:119:GLN:HA   | 1.94                     | 0.97              |
| 1:W:279:GLN:HE21 | 1:W:320:ILE:HG12 | 1.22                     | 0.97              |
| 1:X:357:LYS:HA   | 1:X:367:ILE:HD11 | 1.46                     | 0.97              |
| 2:I:83:ARG:HG2   | 2:J:55:THR:HG22  | 1.46                     | 0.97              |
| 1:S:279:GLN:NE2  | 1:S:320:ILE:HG12 | 1.80                     | 0.96              |
| 2:J:52:ASP:HA    | 2:J:55:THR:HG23  | 1.47                     | 0.96              |
| 2:R:56:LEU:HB2   | 2:R:91:LEU:HD23  | 1.47                     | 0.96              |
| 1:T:357:LYS:HA   | 1:T:367:ILE:HD11 | 1.48                     | 0.96              |
| 1:E:111:VAL:HG21 | 1:E:244:ALA:HA   | 1.47                     | 0.96              |
| 1:U:357:LYS:HA   | 1:U:367:ILE:HD11 | 1.46                     | 0.96              |
| 1:S:357:LYS:HA   | 1:S:367:ILE:HD11 | 1.45                     | 0.95              |
| 1:V:357:LYS:HA   | 1:V:367:ILE:HD11 | 1.47                     | 0.95              |
| 1:V:279:GLN:NE2  | 1:V:320:ILE:HG12 | 1.81                     | 0.95              |
| 2:M:56:LEU:HB2   | 2:M:91:LEU:HD23  | 1.49                     | 0.95              |
| 1:B:264:LYS:HZ1  | 1:B:279:GLN:HE22 | 1.14                     | 0.94              |
| 1:C:406:LYS:H    | 1:C:406:LYS:HD2  | 1.32                     | 0.94              |
| 1:W:357:LYS:HA   | 1:W:367:ILE:HD11 | 1.47                     | 0.94              |
| 1:B:231:ALA:HA   | 1:B:234:LEU:HD21 | 1.48                     | 0.94              |
| 1:C:60:GLY:HA2   | 3:C:452:ATP:O3A  | 1.65                     | 0.94              |
| 1:E:52:ASN:ND2   | 1:E:305:PHE:H    | 1.65                     | 0.94              |
| 1:D:264:LYS:HZ1  | 1:D:279:GLN:HE22 | 1.09                     | 0.93              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:56:LEU:HB2   | 2:O:91:LEU:HD23  | 1.48                     | 0.93              |
| 1:X:279:GLN:NE2  | 1:X:320:ILE:HG12 | 1.83                     | 0.93              |
| 1:U:279:GLN:NE2  | 1:U:320:ILE:HG12 | 1.82                     | 0.93              |
| 1:F:264:LYS:HZ1  | 1:F:279:GLN:NE2  | 1.66                     | 0.92              |
| 1:X:442:PHE:HD1  | 1:X:442:PHE:H    | 1.04                     | 0.92              |
| 2:P:56:LEU:HB2   | 2:P:91:LEU:HD23  | 1.48                     | 0.92              |
| 1:T:437:GLU:HG3  | 1:T:438:ASP:H    | 1.33                     | 0.92              |
| 2:Q:56:LEU:HB2   | 2:Q:91:LEU:HD23  | 1.50                     | 0.92              |
| 1:S:235:ILE:HG22 | 1:S:237:PRO:HD3  | 1.52                     | 0.91              |
| 1:T:279:GLN:NE2  | 1:T:320:ILE:HG12 | 1.84                     | 0.91              |
| 1:V:279:GLN:HE22 | 1:V:320:ILE:H    | 1.14                     | 0.91              |
| 2:K:137:LEU:O    | 2:K:141:THR:HG23 | 1.71                     | 0.91              |
| 2:I:52:ASP:HA    | 2:I:55:THR:HG23  | 1.51                     | 0.90              |
| 2:N:56:LEU:HB2   | 2:N:91:LEU:HD23  | 1.52                     | 0.90              |
| 1:E:406:LYS:H    | 1:E:406:LYS:HD2  | 1.37                     | 0.90              |
| 1:A:366:ASN:HB3  | 1:A:418:THR:HG22 | 1.53                     | 0.90              |
| 1:T:236:ASN:OD1  | 1:T:239:GLU:HB3  | 1.72                     | 0.90              |
| 1:B:409:PHE:CD1  | 1:C:6:PRO:HB3    | 2.07                     | 0.90              |
| 1:X:279:GLN:HE22 | 1:X:320:ILE:H    | 1.17                     | 0.89              |
| 1:W:279:GLN:HE22 | 1:W:320:ILE:H    | 1.18                     | 0.89              |
| 1:T:64:THR:HB    | 3:T:457:ATP:O2A  | 1.73                     | 0.89              |
| 1:E:264:LYS:HZ1  | 1:E:279:GLN:HE22 | 1.16                     | 0.89              |
| 2:Q:7:ARG:CD     | 2:Q:119:GLN:OE1  | 2.21                     | 0.88              |
| 1:W:279:GLN:NE2  | 1:W:320:ILE:HG12 | 1.88                     | 0.88              |
| 2:L:52:ASP:HA    | 2:L:55:THR:HG23  | 1.53                     | 0.88              |
| 1:D:264:LYS:HE3  | 1:D:264:LYS:N    | 1.88                     | 0.88              |
| 1:E:20:GLN:HE21  | 1:E:20:GLN:CA    | 1.86                     | 0.88              |
| 2:Q:131:LEU:HD11 | 2:Q:135:ARG:NE   | 1.88                     | 0.88              |
| 1:A:58:PRO:HD2   | 1:A:61:VAL:HG21  | 1.54                     | 0.88              |
| 1:E:367:ILE:HD11 | 1:E:421:ILE:HD11 | 1.56                     | 0.88              |
| 2:J:144:SER:HB3  | 2:J:147:GLU:HG3  | 1.55                     | 0.88              |
| 2:M:112:VAL:HB   | 1:S:443:ILE:HD12 | 1.55                     | 0.88              |
| 1:U:279:GLN:HE22 | 1:U:320:ILE:H    | 1.16                     | 0.88              |
| 2:R:76:VAL:HG22  | 1:X:443:ILE:HD11 | 1.54                     | 0.87              |
| 2:L:137:LEU:O    | 2:L:141:THR:HG23 | 1.74                     | 0.87              |
| 1:F:23:ALA:HA    | 1:F:331:VAL:HG21 | 1.56                     | 0.87              |
| 1:T:279:GLN:HE22 | 1:T:320:ILE:H    | 1.15                     | 0.87              |
| 1:U:300:THR:O    | 1:U:303:ILE:HG13 | 1.75                     | 0.87              |
| 1:F:264:LYS:NZ   | 1:F:279:GLN:NE2  | 2.22                     | 0.87              |
| 2:I:7:ARG:CD     | 2:I:119:GLN:OE1  | 2.21                     | 0.87              |
| 2:J:91:LEU:N     | 2:J:91:LEU:HD12  | 1.90                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:17:ASP:HB2   | 2:M:164:ASN:ND2  | 1.90                     | 0.86              |
| 1:A:6:PRO:HB3    | 1:F:409:PHE:CD1  | 2.10                     | 0.86              |
| 2:K:83:ARG:HG2   | 2:L:55:THR:HG22  | 1.57                     | 0.86              |
| 1:E:20:GLN:HA    | 1:E:20:GLN:HE21  | 1.40                     | 0.86              |
| 2:G:17:ASP:O     | 2:G:33:LYS:HD2   | 1.75                     | 0.86              |
| 2:J:18:GLY:H     | 2:J:164:ASN:HD21 | 1.22                     | 0.86              |
| 2:N:7:ARG:HD2    | 2:N:119:GLN:NE2  | 1.88                     | 0.86              |
| 2:G:56:LEU:HD13  | 2:G:95:LEU:HG    | 1.56                     | 0.86              |
| 2:H:56:LEU:HD13  | 2:H:95:LEU:HG    | 1.58                     | 0.86              |
| 2:M:115:PRO:HB3  | 2:M:119:GLN:HA   | 1.56                     | 0.86              |
| 2:M:7:ARG:CD     | 2:M:119:GLN:OE1  | 2.23                     | 0.86              |
| 2:Q:17:ASP:HA    | 2:Q:167:PHE:HB3  | 1.58                     | 0.86              |
| 1:S:369:PHE:HE2  | 1:S:421:ILE:HD12 | 1.41                     | 0.85              |
| 2:N:17:ASP:HB2   | 2:N:164:ASN:ND2  | 1.92                     | 0.85              |
| 1:A:409:PHE:CD1  | 1:B:6:PRO:HB3    | 2.12                     | 0.85              |
| 2:L:56:LEU:HD13  | 2:L:95:LEU:HG    | 1.56                     | 0.85              |
| 2:J:91:LEU:H     | 2:J:91:LEU:CD1   | 1.89                     | 0.85              |
| 1:A:435:GLU:HG3  | 1:A:436:ASN:H    | 1.40                     | 0.85              |
| 1:E:443:ILE:HG23 | 2:K:112:VAL:HG23 | 1.59                     | 0.85              |
| 1:S:327:LEU:N    | 1:S:328:PRO:HD3  | 1.92                     | 0.85              |
| 1:D:27:VAL:HB    | 1:D:70:LEU:HD22  | 1.57                     | 0.85              |
| 1:E:116:ILE:HD12 | 1:E:117:ALA:N    | 1.90                     | 0.85              |
| 1:T:369:PHE:HE2  | 1:T:421:ILE:HD12 | 1.42                     | 0.85              |
| 2:O:17:ASP:HB2   | 2:O:164:ASN:ND2  | 1.92                     | 0.84              |
| 1:W:369:PHE:HE2  | 1:W:421:ILE:HD12 | 1.42                     | 0.84              |
| 2:O:18:GLY:H     | 2:O:164:ASN:HD21 | 1.24                     | 0.84              |
| 1:E:443:ILE:HD11 | 2:K:72:LEU:HD11  | 1.59                     | 0.84              |
| 2:H:144:SER:HB3  | 2:H:147:GLU:HG3  | 1.59                     | 0.84              |
| 1:T:327:LEU:N    | 1:T:328:PRO:HD3  | 1.92                     | 0.84              |
| 1:C:264:LYS:HZ1  | 1:C:279:GLN:HE22 | 1.24                     | 0.84              |
| 1:F:433:VAL:HG12 | 1:F:434:VAL:H    | 1.43                     | 0.84              |
| 1:B:111:VAL:HG21 | 1:B:244:ALA:HA   | 1.60                     | 0.84              |
| 1:S:393:ALA:HB3  | 3:S:456:ATP:H1'  | 1.60                     | 0.84              |
| 1:T:442:PHE:HD1  | 1:T:442:PHE:N    | 1.75                     | 0.84              |
| 2:Q:17:ASP:HB2   | 2:Q:164:ASN:ND2  | 1.91                     | 0.84              |
| 1:B:20:GLN:HE21  | 1:B:20:GLN:HA    | 1.42                     | 0.84              |
| 1:A:264:LYS:HZ1  | 1:A:279:GLN:HE22 | 1.25                     | 0.84              |
| 1:W:439:LEU:HG   | 1:W:440:SER:H    | 1.43                     | 0.83              |
| 2:R:17:ASP:HA    | 2:R:167:PHE:HB3  | 1.60                     | 0.83              |
| 2:R:8:ARG:HB3    | 2:R:8:ARG:HH11   | 1.42                     | 0.83              |
| 2:N:8:ARG:HB3    | 2:N:8:ARG:HH11   | 1.42                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:20:GLN:HE21  | 1:B:20:GLN:CA    | 1.90                     | 0.83              |
| 2:H:137:LEU:O    | 2:H:141:THR:HG23 | 1.79                     | 0.83              |
| 2:M:131:LEU:HD11 | 2:M:135:ARG:NE   | 1.93                     | 0.83              |
| 2:O:8:ARG:HB3    | 2:O:8:ARG:HH11   | 1.42                     | 0.83              |
| 2:P:17:ASP:HB2   | 2:P:164:ASN:ND2  | 1.94                     | 0.83              |
| 2:G:37:LEU:HB2   | 2:G:42:VAL:HG23  | 1.60                     | 0.83              |
| 2:M:8:ARG:HH11   | 2:M:8:ARG:HB3    | 1.41                     | 0.83              |
| 2:I:17:ASP:HB2   | 2:I:164:ASN:ND2  | 1.94                     | 0.83              |
| 2:P:17:ASP:HA    | 2:P:167:PHE:HB3  | 1.61                     | 0.83              |
| 1:X:369:PHE:HE2  | 1:X:421:ILE:HD12 | 1.42                     | 0.83              |
| 1:T:442:PHE:H    | 1:T:442:PHE:HD1  | 1.27                     | 0.83              |
| 2:N:7:ARG:CD     | 2:N:119:GLN:NE2  | 2.42                     | 0.83              |
| 2:M:17:ASP:HA    | 2:M:167:PHE:HB3  | 1.60                     | 0.83              |
| 1:U:327:LEU:N    | 1:U:328:PRO:HD3  | 1.92                     | 0.82              |
| 2:G:137:LEU:O    | 2:G:141:THR:HG23 | 1.78                     | 0.82              |
| 2:N:17:ASP:HA    | 2:N:167:PHE:HB3  | 1.61                     | 0.82              |
| 1:F:37:ARG:HD2   | 1:F:48:VAL:HG13  | 1.61                     | 0.82              |
| 1:C:337:SER:HB3  | 1:C:340:ASP:OD2  | 1.77                     | 0.82              |
| 1:W:327:LEU:N    | 1:W:328:PRO:HD3  | 1.92                     | 0.82              |
| 1:D:403:LEU:HD23 | 1:D:404:MET:N    | 1.93                     | 0.82              |
| 2:M:18:GLY:H     | 2:M:164:ASN:HD21 | 1.24                     | 0.82              |
| 1:X:300:THR:O    | 1:X:303:ILE:HG13 | 1.80                     | 0.82              |
| 1:E:52:ASN:ND2   | 1:E:305:PHE:HB2  | 1.95                     | 0.82              |
| 2:O:17:ASP:HA    | 2:O:167:PHE:HB3  | 1.62                     | 0.82              |
| 2:H:88:LEU:O     | 2:H:90:LYS:N     | 2.12                     | 0.82              |
| 1:U:369:PHE:HE2  | 1:U:421:ILE:HD12 | 1.43                     | 0.82              |
| 1:F:403:LEU:HD23 | 1:F:404:MET:N    | 1.95                     | 0.82              |
| 1:E:403:LEU:HD23 | 1:E:404:MET:N    | 1.95                     | 0.82              |
| 2:J:83:ARG:HG2   | 2:K:55:THR:HG22  | 1.62                     | 0.82              |
| 2:Q:8:ARG:HH11   | 2:Q:8:ARG:HB3    | 1.44                     | 0.81              |
| 1:V:434:VAL:HG12 | 1:V:435:GLU:H    | 1.43                     | 0.81              |
| 2:G:17:ASP:HB2   | 2:G:164:ASN:ND2  | 1.95                     | 0.81              |
| 1:X:327:LEU:N    | 1:X:328:PRO:HD3  | 1.95                     | 0.81              |
| 2:R:131:LEU:HD11 | 2:R:135:ARG:NE   | 1.94                     | 0.81              |
| 2:M:115:PRO:HB2  | 2:M:119:GLN:HA   | 1.58                     | 0.81              |
| 2:R:18:GLY:H     | 2:R:164:ASN:HD21 | 1.27                     | 0.81              |
| 1:S:60:GLY:HA3   | 1:S:392:GLY:HA3  | 1.62                     | 0.81              |
| 1:D:275:ARG:C    | 1:D:277:GLY:H    | 1.82                     | 0.81              |
| 2:P:8:ARG:HH11   | 2:P:8:ARG:HB3    | 1.45                     | 0.81              |
| 1:F:264:LYS:HZ1  | 1:F:279:GLN:HE22 | 0.85                     | 0.81              |
| 1:E:264:LYS:N    | 1:E:264:LYS:HE3  | 1.96                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:421:ILE:HG23 | 1:B:425:TYR:CD1  | 2.16                     | 0.81              |
| 2:K:79:ALA:HB1   | 2:K:83:ARG:HH21  | 1.44                     | 0.81              |
| 2:H:18:GLY:H     | 2:H:164:ASN:HD21 | 1.26                     | 0.81              |
| 2:I:83:ARG:HG2   | 2:J:55:THR:CG2   | 2.11                     | 0.81              |
| 1:V:54:LEU:HD21  | 1:V:327:LEU:HD13 | 1.60                     | 0.81              |
| 1:F:337:SER:HB3  | 1:F:340:ASP:OD2  | 1.81                     | 0.81              |
| 1:B:403:LEU:HD23 | 1:B:404:MET:N    | 1.94                     | 0.81              |
| 1:A:236:ASN:ND2  | 1:A:239:GLU:HB2  | 1.96                     | 0.81              |
| 1:T:442:PHE:CD1  | 1:T:442:PHE:N    | 2.47                     | 0.80              |
| 2:L:88:LEU:HD23  | 2:L:89:ARG:H     | 1.43                     | 0.80              |
| 2:R:17:ASP:HB2   | 2:R:164:ASN:ND2  | 1.95                     | 0.80              |
| 1:C:439:LEU:HA   | 1:C:443:ILE:HD12 | 1.62                     | 0.80              |
| 2:G:52:ASP:HA    | 2:G:55:THR:HG23  | 1.64                     | 0.80              |
| 1:S:441:ARG:HB3  | 1:S:442:PHE:HD1  | 1.44                     | 0.80              |
| 2:I:18:GLY:H     | 2:I:164:ASN:HD21 | 1.27                     | 0.80              |
| 2:H:82:TRP:HZ2   | 2:H:91:LEU:HD13  | 1.45                     | 0.80              |
| 2:N:18:GLY:H     | 2:N:164:ASN:HD21 | 1.28                     | 0.80              |
| 2:L:17:ASP:HB2   | 2:L:164:ASN:ND2  | 1.96                     | 0.80              |
| 1:D:79:ILE:HG22  | 1:D:103:LEU:HD13 | 1.63                     | 0.80              |
| 2:G:18:GLY:H     | 2:G:164:ASN:HD21 | 1.28                     | 0.80              |
| 2:K:18:GLY:H     | 2:K:164:ASN:HD21 | 1.26                     | 0.80              |
| 1:B:264:LYS:N    | 1:B:264:LYS:HE3  | 1.97                     | 0.80              |
| 2:J:37:LEU:HB2   | 2:J:42:VAL:HG23  | 1.64                     | 0.80              |
| 2:Q:18:GLY:H     | 2:Q:164:ASN:HD21 | 1.27                     | 0.79              |
| 2:I:144:SER:HB3  | 2:I:147:GLU:HG3  | 1.63                     | 0.79              |
| 1:T:54:LEU:HD21  | 1:T:327:LEU:HD13 | 1.64                     | 0.79              |
| 2:R:5:SER:HB2    | 2:R:14:VAL:HG22  | 1.63                     | 0.79              |
| 1:X:77:PRO:HD2   | 1:X:251:ASN:O    | 1.82                     | 0.79              |
| 1:V:77:PRO:HD2   | 1:V:251:ASN:O    | 1.81                     | 0.79              |
| 2:Q:131:LEU:HD11 | 2:Q:135:ARG:HE   | 1.47                     | 0.79              |
| 2:G:144:SER:HB3  | 2:G:147:GLU:HG3  | 1.65                     | 0.79              |
| 1:V:327:LEU:N    | 1:V:328:PRO:HD3  | 1.95                     | 0.79              |
| 1:S:279:GLN:HE22 | 1:S:320:ILE:N    | 1.81                     | 0.79              |
| 1:X:54:LEU:HD21  | 1:X:327:LEU:HD13 | 1.65                     | 0.79              |
| 2:P:131:LEU:HD11 | 2:P:135:ARG:NE   | 1.96                     | 0.79              |
| 1:T:260:ASP:HB3  | 1:T:311:PHE:CD2  | 2.18                     | 0.79              |
| 1:U:77:PRO:HD2   | 1:U:251:ASN:O    | 1.83                     | 0.79              |
| 2:K:144:SER:HB3  | 2:K:147:GLU:HG3  | 1.65                     | 0.79              |
| 1:W:260:ASP:HB3  | 1:W:311:PHE:CD2  | 2.18                     | 0.79              |
| 2:G:105:ILE:CG2  | 2:G:113:VAL:HB   | 2.13                     | 0.79              |
| 1:F:57:GLY:O     | 1:F:310:ALA:HA   | 1.83                     | 0.78              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:38:TYR:CE1   | 2:L:69:GLY:HA3   | 2.18                     | 0.78              |
| 1:X:64:THR:HB    | 3:X:461:ATP:O2A  | 1.83                     | 0.78              |
| 1:V:369:PHE:HE2  | 1:V:421:ILE:HD12 | 1.46                     | 0.78              |
| 2:M:131:LEU:HD11 | 2:M:135:ARG:HE   | 1.49                     | 0.78              |
| 2:M:164:ASN:HD22 | 2:M:164:ASN:H    | 1.30                     | 0.78              |
| 1:W:54:LEU:HD21  | 1:W:327:LEU:HD13 | 1.65                     | 0.78              |
| 1:E:27:VAL:HB    | 1:E:70:LEU:HD22  | 1.64                     | 0.78              |
| 1:F:441:ARG:NH2  | 2:G:37:LEU:HA    | 1.99                     | 0.78              |
| 2:H:52:ASP:HA    | 2:H:55:THR:HG23  | 1.65                     | 0.78              |
| 2:M:55:THR:HG22  | 2:N:83:ARG:HG2   | 1.66                     | 0.78              |
| 1:D:440:SER:O    | 1:D:442:PHE:N    | 2.16                     | 0.78              |
| 1:A:403:LEU:HD23 | 1:A:404:MET:N    | 1.99                     | 0.78              |
| 2:O:5:SER:HB2    | 2:O:14:VAL:HG22  | 1.65                     | 0.78              |
| 2:M:42:VAL:HG12  | 2:M:99:ASP:HB3   | 1.66                     | 0.78              |
| 1:F:104:THR:HA   | 1:F:248:VAL:HG21 | 1.65                     | 0.78              |
| 1:S:260:ASP:HB3  | 1:S:311:PHE:CD2  | 2.19                     | 0.78              |
| 1:T:96:VAL:HG13  | 1:T:282:LEU:HD12 | 1.66                     | 0.78              |
| 1:B:337:SER:HB3  | 1:B:340:ASP:OD2  | 1.82                     | 0.78              |
| 1:S:77:PRO:HD2   | 1:S:251:ASN:O    | 1.83                     | 0.78              |
| 1:T:303:ILE:HG22 | 1:T:304:LEU:H    | 1.49                     | 0.78              |
| 1:C:264:LYS:HE3  | 1:C:264:LYS:N    | 1.97                     | 0.78              |
| 1:S:96:VAL:HG13  | 1:S:282:LEU:HD12 | 1.65                     | 0.78              |
| 1:E:280:ARG:HG3  | 1:E:280:ARG:HH11 | 1.47                     | 0.78              |
| 1:C:23:ALA:HA    | 1:C:331:VAL:HG21 | 1.66                     | 0.78              |
| 1:C:52:ASN:O     | 1:C:328:PRO:HD2  | 1.82                     | 0.78              |
| 1:B:60:GLY:HA2   | 3:B:451:ATP:O3A  | 1.84                     | 0.78              |
| 1:D:37:ARG:HD2   | 1:D:48:VAL:HG13  | 1.66                     | 0.78              |
| 1:U:303:ILE:HG22 | 1:U:304:LEU:H    | 1.47                     | 0.77              |
| 2:K:17:ASP:HB2   | 2:K:164:ASN:ND2  | 1.99                     | 0.77              |
| 2:J:118:ASP:O    | 2:J:119:GLN:O    | 2.02                     | 0.77              |
| 1:V:300:THR:O    | 1:V:303:ILE:HG13 | 1.83                     | 0.77              |
| 2:Q:5:SER:HB2    | 2:Q:14:VAL:HG22  | 1.66                     | 0.77              |
| 1:T:300:THR:O    | 1:T:303:ILE:HG13 | 1.83                     | 0.77              |
| 1:V:96:VAL:HG13  | 1:V:282:LEU:HD12 | 1.66                     | 0.77              |
| 1:D:58:PRO:O     | 1:D:63:LYS:NZ    | 2.17                     | 0.77              |
| 2:L:91:LEU:O     | 2:L:108:GLY:HA3  | 1.85                     | 0.77              |
| 1:V:260:ASP:HB3  | 1:V:311:PHE:CD2  | 2.20                     | 0.77              |
| 1:F:403:LEU:C    | 1:F:403:LEU:HD23 | 2.04                     | 0.77              |
| 1:C:52:ASN:HD22  | 1:C:305:PHE:H    | 1.27                     | 0.77              |
| 2:P:5:SER:HB2    | 2:P:14:VAL:HG22  | 1.67                     | 0.77              |
| 2:H:7:ARG:HD2    | 2:H:119:GLN:OE1  | 1.85                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:264:LYS:N    | 1:A:264:LYS:HE3  | 2.00                     | 0.77              |
| 1:X:227:ILE:HG23 | 1:X:228:ASP:H    | 1.49                     | 0.77              |
| 2:P:18:GLY:H     | 2:P:164:ASN:HD21 | 1.31                     | 0.77              |
| 1:T:77:PRO:HD2   | 1:T:251:ASN:O    | 1.84                     | 0.77              |
| 1:D:242:GLN:HA   | 1:D:245:ILE:HD12 | 1.66                     | 0.77              |
| 1:X:260:ASP:HB3  | 1:X:311:PHE:CD2  | 2.19                     | 0.77              |
| 2:M:116:GLU:O    | 2:M:119:GLN:N    | 2.11                     | 0.77              |
| 2:N:131:LEU:HD11 | 2:N:135:ARG:NE   | 2.00                     | 0.77              |
| 1:D:20:GLN:H     | 1:D:20:GLN:HE21  | 1.31                     | 0.77              |
| 1:E:79:ILE:HG22  | 1:E:103:LEU:HD13 | 1.67                     | 0.77              |
| 1:U:313:VAL:HG23 | 1:U:314:ALA:N    | 1.99                     | 0.77              |
| 1:A:37:ARG:HD2   | 1:A:48:VAL:HG13  | 1.65                     | 0.77              |
| 2:P:42:VAL:HG12  | 2:P:99:ASP:HB3   | 1.66                     | 0.77              |
| 1:T:439:LEU:O    | 1:T:441:ARG:N    | 2.18                     | 0.76              |
| 1:W:300:THR:O    | 1:W:303:ILE:HG13 | 1.84                     | 0.76              |
| 1:B:362:THR:CG2  | 1:C:39:GLN:HG2   | 2.14                     | 0.76              |
| 1:A:264:LYS:HZ3  | 1:A:279:GLN:HE22 | 1.29                     | 0.76              |
| 1:S:439:LEU:HD23 | 1:S:439:LEU:H    | 1.51                     | 0.76              |
| 1:C:443:ILE:HD11 | 2:I:72:LEU:HD11  | 1.64                     | 0.76              |
| 2:H:105:ILE:CG2  | 2:H:113:VAL:HB   | 2.16                     | 0.76              |
| 1:F:36:ARG:O     | 1:F:39:GLN:HB3   | 1.86                     | 0.76              |
| 1:S:300:THR:O    | 1:S:303:ILE:HG13 | 1.84                     | 0.76              |
| 1:S:65:GLU:HG2   | 3:S:456:ATP:H5'2 | 1.66                     | 0.76              |
| 2:R:164:ASN:H    | 2:R:164:ASN:HD22 | 1.33                     | 0.76              |
| 1:U:54:LEU:HD21  | 1:U:327:LEU:HD13 | 1.67                     | 0.76              |
| 2:L:18:GLY:H     | 2:L:164:ASN:HD21 | 1.27                     | 0.76              |
| 2:J:105:ILE:CG2  | 2:J:113:VAL:HB   | 2.14                     | 0.76              |
| 2:Q:164:ASN:HD22 | 2:Q:164:ASN:H    | 1.33                     | 0.76              |
| 2:O:164:ASN:H    | 2:O:164:ASN:HD22 | 1.34                     | 0.76              |
| 1:B:23:ALA:HA    | 1:B:331:VAL:HG21 | 1.67                     | 0.76              |
| 1:A:337:SER:HB3  | 1:A:340:ASP:OD2  | 1.86                     | 0.76              |
| 1:D:352:LEU:HD13 | 1:D:400:MET:HG3  | 1.67                     | 0.76              |
| 1:U:260:ASP:HB3  | 1:U:311:PHE:CD2  | 2.21                     | 0.76              |
| 2:O:42:VAL:HG12  | 2:O:99:ASP:HB3   | 1.68                     | 0.76              |
| 2:N:103:SER:O    | 2:N:104:LEU:HD23 | 1.86                     | 0.76              |
| 1:S:54:LEU:HD21  | 1:S:327:LEU:HD13 | 1.67                     | 0.76              |
| 1:W:313:VAL:HG23 | 1:W:314:ALA:N    | 2.00                     | 0.76              |
| 2:O:131:LEU:HD11 | 2:O:135:ARG:NE   | 2.01                     | 0.76              |
| 1:D:17:ILE:HD12  | 1:D:17:ILE:N     | 2.02                     | 0.75              |
| 1:W:326:ARG:HH11 | 1:W:326:ARG:HB3  | 1.52                     | 0.75              |
| 1:X:313:VAL:HG23 | 1:X:314:ALA:N    | 2.00                     | 0.75              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:405:ASP:HB3  | 1:A:406:LYS:HD2  | 1.68                     | 0.75              |
| 1:T:313:VAL:HG23 | 1:T:314:ALA:N    | 1.98                     | 0.75              |
| 2:R:42:VAL:HG12  | 2:R:99:ASP:HB3   | 1.69                     | 0.75              |
| 2:G:57:PHE:HA    | 2:G:95:LEU:HD11  | 1.68                     | 0.75              |
| 2:L:88:LEU:HD23  | 2:L:89:ARG:N     | 2.00                     | 0.75              |
| 1:A:275:ARG:C    | 1:A:277:GLY:H    | 1.88                     | 0.75              |
| 2:L:52:ASP:CA    | 2:L:55:THR:HG23  | 2.16                     | 0.75              |
| 1:E:275:ARG:C    | 1:E:277:GLY:H    | 1.88                     | 0.75              |
| 2:O:76:VAL:HG11  | 1:U:442:PHE:HD2  | 1.52                     | 0.75              |
| 1:E:64:THR:HB    | 3:E:454:ATP:O1A  | 1.86                     | 0.75              |
| 1:W:303:ILE:HG22 | 1:W:304:LEU:H    | 1.52                     | 0.75              |
| 1:U:96:VAL:HG13  | 1:U:282:LEU:HD12 | 1.67                     | 0.75              |
| 2:N:7:ARG:NE     | 2:N:119:GLN:NE2  | 2.33                     | 0.75              |
| 1:S:393:ALA:CB   | 3:S:456:ATP:H1'  | 2.16                     | 0.75              |
| 2:K:52:ASP:HA    | 2:K:55:THR:HG23  | 1.69                     | 0.75              |
| 1:B:104:THR:HA   | 1:B:248:VAL:HG21 | 1.69                     | 0.75              |
| 2:K:105:ILE:CG2  | 2:K:113:VAL:HB   | 2.15                     | 0.75              |
| 2:G:105:ILE:HG23 | 2:G:113:VAL:HB   | 1.68                     | 0.75              |
| 1:A:233:LYS:HD2  | 1:A:234:LEU:N    | 2.02                     | 0.74              |
| 1:D:367:ILE:HD11 | 1:D:421:ILE:HD11 | 1.69                     | 0.74              |
| 1:F:17:ILE:N     | 1:F:17:ILE:HD12  | 2.03                     | 0.74              |
| 1:V:303:ILE:HG22 | 1:V:304:LEU:H    | 1.50                     | 0.74              |
| 1:B:366:ASN:HB3  | 1:B:418:THR:HG22 | 1.67                     | 0.74              |
| 1:U:279:GLN:HE22 | 1:U:320:ILE:N    | 1.85                     | 0.74              |
| 1:C:435:GLU:HG2  | 1:C:436:ASN:H    | 1.51                     | 0.74              |
| 1:D:407:ILE:O    | 1:D:411:ALA:HB2  | 1.87                     | 0.74              |
| 1:W:96:VAL:HG13  | 1:W:282:LEU:HD12 | 1.67                     | 0.74              |
| 1:B:275:ARG:C    | 1:B:277:GLY:H    | 1.90                     | 0.74              |
| 1:B:232:ALA:H    | 1:B:234:LEU:HD23 | 1.52                     | 0.74              |
| 1:F:441:ARG:HH22 | 2:G:37:LEU:HA    | 1.53                     | 0.74              |
| 1:C:104:THR:HA   | 1:C:248:VAL:HG21 | 1.68                     | 0.74              |
| 2:G:13:VAL:HG22  | 2:G:171:GLU:HB3  | 1.70                     | 0.74              |
| 1:V:326:ARG:HH11 | 1:V:326:ARG:HB3  | 1.51                     | 0.74              |
| 1:S:6:PRO:HD3    | 1:S:32:ARG:HD3   | 1.70                     | 0.74              |
| 1:D:264:LYS:NZ   | 1:D:279:GLN:NE2  | 2.34                     | 0.74              |
| 1:X:279:GLN:HE22 | 1:X:320:ILE:N    | 1.86                     | 0.74              |
| 1:B:36:ARG:O     | 1:B:39:GLN:HB3   | 1.87                     | 0.74              |
| 2:I:82:TRP:HZ2   | 2:I:91:LEU:HD23  | 1.51                     | 0.74              |
| 2:L:37:LEU:HD21  | 2:L:57:PHE:CZ    | 2.21                     | 0.74              |
| 2:G:13:VAL:HG22  | 2:G:171:GLU:CB   | 2.18                     | 0.74              |
| 1:B:5:THR:H      | 1:B:8:GLU:HB3    | 1.53                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:442:PHE:O    | 1:T:443:ILE:HG12 | 1.88                     | 0.73              |
| 1:V:279:GLN:HE22 | 1:V:320:ILE:N    | 1.84                     | 0.73              |
| 1:V:313:VAL:HG23 | 1:V:314:ALA:N    | 1.99                     | 0.73              |
| 1:B:232:ALA:H    | 1:B:234:LEU:CD2  | 2.01                     | 0.73              |
| 1:B:79:ILE:HG22  | 1:B:103:LEU:HD13 | 1.70                     | 0.73              |
| 1:D:104:THR:HA   | 1:D:248:VAL:HG21 | 1.68                     | 0.73              |
| 1:X:96:VAL:HG13  | 1:X:282:LEU:HD12 | 1.68                     | 0.73              |
| 1:F:264:LYS:N    | 1:F:264:LYS:HE3  | 2.03                     | 0.73              |
| 2:P:164:ASN:HD22 | 2:P:164:ASN:H    | 1.34                     | 0.73              |
| 1:B:352:LEU:HD13 | 1:B:400:MET:HG3  | 1.68                     | 0.73              |
| 1:W:6:PRO:HD3    | 1:W:32:ARG:HD3   | 1.70                     | 0.73              |
| 2:G:37:LEU:HD21  | 2:G:57:PHE:CZ    | 2.23                     | 0.73              |
| 1:D:36:ARG:O     | 1:D:39:GLN:HB3   | 1.88                     | 0.73              |
| 1:C:403:LEU:C    | 1:C:403:LEU:HD23 | 2.08                     | 0.73              |
| 1:A:83:ALA:HB1   | 1:A:262:ILE:HD13 | 1.69                     | 0.73              |
| 1:X:395:ARG:O    | 1:X:399:VAL:HG23 | 1.89                     | 0.73              |
| 1:E:367:ILE:HD11 | 1:E:421:ILE:CD1  | 2.19                     | 0.73              |
| 2:H:17:ASP:HB2   | 2:H:164:ASN:ND2  | 2.03                     | 0.73              |
| 1:E:37:ARG:HD2   | 1:E:48:VAL:HG13  | 1.69                     | 0.73              |
| 2:H:91:LEU:CD1   | 2:H:91:LEU:H     | 2.02                     | 0.73              |
| 1:S:303:ILE:HG22 | 1:S:304:LEU:H    | 1.52                     | 0.73              |
| 1:F:20:GLN:CA    | 1:F:20:GLN:HE21  | 2.01                     | 0.73              |
| 1:U:326:ARG:HB3  | 1:U:326:ARG:HH11 | 1.54                     | 0.73              |
| 2:O:103:SER:O    | 2:O:104:LEU:HD23 | 1.87                     | 0.73              |
| 1:V:395:ARG:O    | 1:V:399:VAL:HG23 | 1.88                     | 0.73              |
| 2:Q:42:VAL:HG12  | 2:Q:99:ASP:HB3   | 1.70                     | 0.73              |
| 2:R:103:SER:O    | 2:R:104:LEU:HD23 | 1.89                     | 0.73              |
| 2:L:46:PHE:HB3   | 2:L:95:LEU:CD2   | 2.19                     | 0.73              |
| 1:W:77:PRO:HD2   | 1:W:251:ASN:O    | 1.87                     | 0.73              |
| 1:F:37:ARG:HH12  | 1:F:38:MET:HE2   | 1.53                     | 0.73              |
| 1:X:303:ILE:HG22 | 1:X:304:LEU:H    | 1.53                     | 0.73              |
| 1:T:6:PRO:HD3    | 1:T:32:ARG:HD3   | 1.71                     | 0.73              |
| 1:C:403:LEU:HD23 | 1:C:404:MET:N    | 2.03                     | 0.73              |
| 1:T:326:ARG:HH11 | 1:T:326:ARG:HB3  | 1.54                     | 0.73              |
| 1:E:264:LYS:HZ3  | 1:E:279:GLN:HE22 | 1.36                     | 0.72              |
| 1:A:367:ILE:HD11 | 1:A:421:ILE:HD11 | 1.68                     | 0.72              |
| 1:D:116:ILE:HD12 | 1:D:117:ALA:N    | 2.04                     | 0.72              |
| 1:D:409:PHE:CD1  | 1:E:6:PRO:HB3    | 2.24                     | 0.72              |
| 1:F:79:ILE:HG22  | 1:F:103:LEU:HD13 | 1.70                     | 0.72              |
| 2:I:37:LEU:HB2   | 2:I:42:VAL:HG23  | 1.70                     | 0.72              |
| 1:X:6:PRO:HD3    | 1:X:32:ARG:HD3   | 1.71                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:103:SER:O    | 2:Q:104:LEU:HD23 | 1.89                     | 0.72              |
| 1:S:313:VAL:HG23 | 1:S:314:ALA:N    | 2.00                     | 0.72              |
| 1:W:279:GLN:HE22 | 1:W:320:ILE:N    | 1.87                     | 0.72              |
| 2:N:42:VAL:HG12  | 2:N:99:ASP:HB3   | 1.70                     | 0.72              |
| 1:A:39:GLN:HG2   | 1:F:362:THR:CG2  | 2.18                     | 0.72              |
| 1:F:443:ILE:HD11 | 2:L:72:LEU:HD11  | 1.72                     | 0.72              |
| 1:U:6:PRO:HD3    | 1:U:32:ARG:HD3   | 1.69                     | 0.72              |
| 1:C:5:THR:H      | 1:C:8:GLU:HB3    | 1.55                     | 0.72              |
| 2:L:144:SER:HB3  | 2:L:147:GLU:HG3  | 1.69                     | 0.72              |
| 1:A:362:THR:CG2  | 1:B:39:GLN:HG2   | 2.20                     | 0.72              |
| 2:R:131:LEU:HD11 | 2:R:135:ARG:HE   | 1.53                     | 0.72              |
| 1:C:5:THR:O      | 1:C:9:ILE:HG13   | 1.89                     | 0.72              |
| 1:B:283:LEU:HB2  | 1:B:284:PRO:HD3  | 1.70                     | 0.72              |
| 1:S:326:ARG:HH11 | 1:S:326:ARG:HB3  | 1.55                     | 0.72              |
| 2:K:83:ARG:HG2   | 2:L:55:THR:CG2   | 2.19                     | 0.72              |
| 1:D:20:GLN:HE21  | 1:D:20:GLN:N     | 1.87                     | 0.72              |
| 1:E:108:MET:HG3  | 1:E:295:HIS:CE1  | 2.24                     | 0.72              |
| 2:K:56:LEU:HD13  | 2:K:95:LEU:HG    | 1.72                     | 0.72              |
| 1:E:415:ASN:OD1  | 1:E:416:GLY:N    | 2.22                     | 0.72              |
| 1:V:442:PHE:O    | 1:V:443:ILE:HG12 | 1.90                     | 0.72              |
| 1:A:421:ILE:HG23 | 1:A:425:TYR:CD1  | 2.25                     | 0.72              |
| 1:A:52:ASN:O     | 1:A:328:PRO:HD2  | 1.90                     | 0.72              |
| 1:X:235:ILE:O    | 1:X:236:ASN:HB2  | 1.90                     | 0.72              |
| 1:E:421:ILE:HA   | 1:E:425:TYR:HD1  | 1.55                     | 0.72              |
| 1:E:362:THR:CG2  | 1:F:39:GLN:HG2   | 2.20                     | 0.72              |
| 2:K:37:LEU:HD21  | 2:K:57:PHE:CZ    | 2.25                     | 0.72              |
| 1:F:275:ARG:C    | 1:F:277:GLY:H    | 1.93                     | 0.72              |
| 1:T:279:GLN:HE22 | 1:T:320:ILE:N    | 1.85                     | 0.71              |
| 1:F:38:MET:HG3   | 1:F:45:ARG:NH1   | 2.05                     | 0.71              |
| 1:W:328:PRO:HB3  | 1:X:398:THR:HA   | 1.72                     | 0.71              |
| 1:E:366:ASN:HB3  | 1:E:418:THR:HG22 | 1.72                     | 0.71              |
| 1:E:264:LYS:NZ   | 1:E:279:GLN:NE2  | 2.28                     | 0.71              |
| 1:U:395:ARG:O    | 1:U:399:VAL:HG23 | 1.89                     | 0.71              |
| 1:X:326:ARG:HH11 | 1:X:326:ARG:HB3  | 1.54                     | 0.71              |
| 1:A:408:SER:O    | 1:B:36:ARG:NH2   | 2.22                     | 0.71              |
| 2:G:37:LEU:HB2   | 2:G:42:VAL:CG2   | 2.20                     | 0.71              |
| 1:S:105:ASP:HB3  | 1:X:297:MET:CE   | 2.20                     | 0.71              |
| 2:N:5:SER:HB2    | 2:N:14:VAL:HG22  | 1.72                     | 0.71              |
| 2:I:91:LEU:HD22  | 2:I:91:LEU:H     | 1.54                     | 0.71              |
| 2:J:37:LEU:HB2   | 2:J:42:VAL:CG2   | 2.20                     | 0.71              |
| 1:A:391:ILE:HG22 | 1:B:321:PRO:HB3  | 1.70                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:63:LYS:HB2   | 3:B:451:ATP:O2B  | 1.90                     | 0.71              |
| 2:N:164:ASN:HD22 | 2:N:164:ASN:H    | 1.38                     | 0.71              |
| 2:P:131:LEU:HD11 | 2:P:135:ARG:HE   | 1.53                     | 0.71              |
| 2:I:137:LEU:O    | 2:I:141:THR:HG23 | 1.90                     | 0.71              |
| 1:D:443:ILE:HG12 | 2:J:112:VAL:HG21 | 1.72                     | 0.71              |
| 1:D:20:GLN:OE1   | 1:D:333:LEU:HB3  | 1.90                     | 0.71              |
| 1:C:100:ILE:HB   | 1:C:291:VAL:HG21 | 1.73                     | 0.71              |
| 2:J:137:LEU:CD1  | 2:P:136:ALA:HB1  | 2.21                     | 0.71              |
| 1:C:256:ILE:HG21 | 1:C:259:ILE:HD12 | 1.70                     | 0.71              |
| 1:A:104:THR:HA   | 1:A:248:VAL:HG21 | 1.72                     | 0.71              |
| 1:S:261:LYS:HE3  | 1:X:280:ARG:HH22 | 1.53                     | 0.71              |
| 2:M:5:SER:HB2    | 2:M:14:VAL:HG22  | 1.71                     | 0.71              |
| 2:L:57:PHE:HA    | 2:L:95:LEU:HD11  | 1.70                     | 0.71              |
| 1:V:6:PRO:HD3    | 1:V:32:ARG:HD3   | 1.71                     | 0.71              |
| 1:T:108:MET:O    | 1:T:112:ARG:HB3  | 1.90                     | 0.71              |
| 1:C:79:ILE:CG2   | 1:C:103:LEU:HD13 | 2.19                     | 0.70              |
| 2:I:57:PHE:HA    | 2:I:95:LEU:HD11  | 1.73                     | 0.70              |
| 1:D:403:LEU:HD23 | 1:D:403:LEU:C    | 2.11                     | 0.70              |
| 1:C:409:PHE:CD1  | 1:D:6:PRO:HB3    | 2.26                     | 0.70              |
| 1:B:100:ILE:HB   | 1:B:291:VAL:HG21 | 1.73                     | 0.70              |
| 1:A:100:ILE:HB   | 1:A:291:VAL:HG21 | 1.72                     | 0.70              |
| 2:G:82:TRP:CZ2   | 2:G:88:LEU:HD22  | 2.25                     | 0.70              |
| 1:A:406:LYS:N    | 1:A:406:LYS:HD2  | 2.04                     | 0.70              |
| 1:S:37:ARG:HH21  | 1:S:302:HIS:CE1  | 2.08                     | 0.70              |
| 1:C:435:GLU:HG2  | 1:C:436:ASN:N    | 2.05                     | 0.70              |
| 2:P:103:SER:O    | 2:P:104:LEU:HD23 | 1.92                     | 0.70              |
| 2:J:17:ASP:HB2   | 2:J:164:ASN:ND2  | 2.07                     | 0.70              |
| 2:I:42:VAL:HG12  | 2:I:99:ASP:HB3   | 1.72                     | 0.70              |
| 1:F:443:ILE:HG12 | 2:L:112:VAL:HG21 | 1.73                     | 0.70              |
| 2:N:137:LEU:O    | 2:N:141:THR:HG22 | 1.91                     | 0.70              |
| 2:P:55:THR:HG22  | 2:Q:83:ARG:HG2   | 1.73                     | 0.70              |
| 1:A:367:ILE:HD11 | 1:A:421:ILE:CD1  | 2.22                     | 0.70              |
| 2:Q:118:ASP:O    | 2:Q:119:GLN:HB2  | 1.92                     | 0.70              |
| 1:A:235:ILE:HG22 | 1:A:237:PRO:HD3  | 1.72                     | 0.70              |
| 1:W:347:GLU:HB2  | 1:W:348:PRO:HD3  | 1.74                     | 0.70              |
| 1:D:83:ALA:HB1   | 1:D:262:ILE:HD13 | 1.73                     | 0.70              |
| 1:W:60:GLY:HA3   | 1:W:392:GLY:HA3  | 1.72                     | 0.70              |
| 1:F:366:ASN:HB3  | 1:F:418:THR:HG22 | 1.74                     | 0.70              |
| 1:C:421:ILE:HG23 | 1:C:425:TYR:CD1  | 2.26                     | 0.70              |
| 1:S:395:ARG:O    | 1:S:399:VAL:HG23 | 1.91                     | 0.70              |
| 1:S:109:LYS:O    | 1:S:113:GLN:HB3  | 1.92                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:23:ALA:HA    | 1:U:331:VAL:HG21 | 1.74                     | 0.70              |
| 1:C:52:ASN:ND2   | 1:C:305:PHE:HB2  | 2.07                     | 0.70              |
| 2:N:105:ILE:HG23 | 2:N:113:VAL:HB   | 1.74                     | 0.70              |
| 2:O:60:PHE:CE2   | 2:O:97:VAL:HG11  | 2.26                     | 0.70              |
| 1:X:313:VAL:CG2  | 1:X:314:ALA:H    | 2.02                     | 0.69              |
| 1:C:37:ARG:HD2   | 1:C:48:VAL:HG13  | 1.74                     | 0.69              |
| 1:T:395:ARG:O    | 1:T:399:VAL:HG23 | 1.92                     | 0.69              |
| 1:E:52:ASN:HD22  | 1:E:305:PHE:H    | 1.36                     | 0.69              |
| 2:Q:137:LEU:O    | 2:Q:141:THR:HG22 | 1.91                     | 0.69              |
| 1:E:104:THR:HA   | 1:E:248:VAL:HG21 | 1.73                     | 0.69              |
| 1:U:385:ASN:HD21 | 1:U:395:ARG:HE   | 1.40                     | 0.69              |
| 1:X:42:GLU:HB3   | 1:X:43:PRO:HD3   | 1.75                     | 0.69              |
| 2:J:52:ASP:CA    | 2:J:55:THR:HG23  | 2.21                     | 0.69              |
| 1:F:405:ASP:HB3  | 1:F:406:LYS:HD2  | 1.74                     | 0.69              |
| 1:T:235:ILE:HG22 | 1:T:237:PRO:HD3  | 1.75                     | 0.69              |
| 1:A:57:GLY:O     | 1:A:310:ALA:HA   | 1.92                     | 0.69              |
| 2:L:37:LEU:HB2   | 2:L:42:VAL:HG23  | 1.73                     | 0.69              |
| 1:D:37:ARG:HA    | 1:D:40:LEU:CD1   | 2.22                     | 0.69              |
| 1:A:403:LEU:C    | 1:A:403:LEU:HD23 | 2.13                     | 0.69              |
| 2:I:105:ILE:HG23 | 2:I:113:VAL:HB   | 1.74                     | 0.69              |
| 1:W:395:ARG:O    | 1:W:399:VAL:HG23 | 1.91                     | 0.69              |
| 1:E:5:THR:H      | 1:E:8:GLU:HB3    | 1.57                     | 0.69              |
| 1:F:100:ILE:HB   | 1:F:291:VAL:HG21 | 1.74                     | 0.69              |
| 1:T:23:ALA:HA    | 1:T:331:VAL:HG21 | 1.74                     | 0.69              |
| 2:G:137:LEU:CD1  | 2:M:136:ALA:HB1  | 2.22                     | 0.69              |
| 2:I:105:ILE:CG2  | 2:I:113:VAL:HB   | 2.23                     | 0.69              |
| 2:I:37:LEU:HD21  | 2:I:57:PHE:CZ    | 2.27                     | 0.69              |
| 1:U:347:GLU:HB2  | 1:U:348:PRO:HD3  | 1.74                     | 0.69              |
| 2:G:38:TYR:CE1   | 2:G:69:GLY:HA3   | 2.27                     | 0.69              |
| 1:F:444:LEU:HD23 | 1:F:444:LEU:C    | 2.12                     | 0.69              |
| 2:H:37:LEU:HD21  | 2:H:57:PHE:CZ    | 2.28                     | 0.69              |
| 1:E:57:GLY:O     | 1:E:310:ALA:HA   | 1.92                     | 0.69              |
| 1:T:347:GLU:HB2  | 1:T:348:PRO:HD3  | 1.75                     | 0.69              |
| 1:V:279:GLN:NE2  | 1:V:320:ILE:N    | 2.40                     | 0.69              |
| 1:U:64:THR:HG1   | 1:U:255:PHE:HE2  | 1.40                     | 0.69              |
| 1:X:63:LYS:HB2   | 3:X:461:ATP:O2B  | 1.93                     | 0.69              |
| 1:D:64:THR:HB    | 3:D:453:ATP:O1A  | 1.92                     | 0.69              |
| 1:W:37:ARG:HH21  | 1:W:302:HIS:CE1  | 2.11                     | 0.69              |
| 2:J:137:LEU:O    | 2:J:141:THR:HG23 | 1.93                     | 0.69              |
| 1:V:5:THR:O      | 1:V:9:ILE:HG13   | 1.92                     | 0.69              |
| 1:U:120:ARG:CD   | 1:U:232:ALA:HA   | 2.23                     | 0.69              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:38:TYR:CE1   | 2:K:69:GLY:HA3   | 2.28                     | 0.69              |
| 2:O:20:VAL:CG2   | 1:V:444:LEU:HD21 | 2.20                     | 0.69              |
| 1:U:37:ARG:HH21  | 1:U:302:HIS:CE1  | 2.11                     | 0.69              |
| 2:H:91:LEU:HD12  | 2:H:91:LEU:H     | 1.57                     | 0.69              |
| 1:V:37:ARG:HH21  | 1:V:302:HIS:CE1  | 2.11                     | 0.69              |
| 1:T:5:THR:O      | 1:T:9:ILE:HG13   | 1.93                     | 0.69              |
| 1:E:264:LYS:HZ1  | 1:E:279:GLN:NE2  | 1.90                     | 0.68              |
| 2:H:105:ILE:HG23 | 2:H:113:VAL:HB   | 1.75                     | 0.68              |
| 2:K:37:LEU:HB2   | 2:K:42:VAL:HG23  | 1.75                     | 0.68              |
| 1:D:23:ALA:HA    | 1:D:331:VAL:HG21 | 1.75                     | 0.68              |
| 1:A:5:THR:H      | 1:A:8:GLU:HB3    | 1.57                     | 0.68              |
| 1:C:36:ARG:O     | 1:C:39:GLN:HB3   | 1.93                     | 0.68              |
| 1:D:367:ILE:HD11 | 1:D:421:ILE:CD1  | 2.24                     | 0.68              |
| 1:E:409:PHE:CD1  | 1:F:6:PRO:HB3    | 2.28                     | 0.68              |
| 1:B:435:GLU:HG2  | 1:B:436:ASN:N    | 2.07                     | 0.68              |
| 1:F:111:VAL:O    | 1:F:114:GLN:HG2  | 1.93                     | 0.68              |
| 2:I:13:VAL:HG22  | 2:I:171:GLU:CB   | 2.22                     | 0.68              |
| 1:C:351:SER:O    | 1:C:355:GLN:HG3  | 1.94                     | 0.68              |
| 1:A:37:ARG:HA    | 1:A:40:LEU:CD1   | 2.24                     | 0.68              |
| 1:B:37:ARG:HD2   | 1:B:48:VAL:HG13  | 1.75                     | 0.68              |
| 1:V:23:ALA:HA    | 1:V:331:VAL:HG21 | 1.75                     | 0.68              |
| 1:C:52:ASN:ND2   | 1:C:305:PHE:N    | 2.38                     | 0.68              |
| 1:X:23:ALA:HA    | 1:X:331:VAL:HG21 | 1.74                     | 0.68              |
| 1:W:5:THR:O      | 1:W:9:ILE:HG13   | 1.94                     | 0.68              |
| 2:K:120:ILE:HD11 | 2:K:138:VAL:HG21 | 1.74                     | 0.68              |
| 1:W:23:ALA:HA    | 1:W:331:VAL:HG21 | 1.74                     | 0.68              |
| 1:X:64:THR:HG1   | 1:X:255:PHE:HE2  | 1.41                     | 0.68              |
| 1:D:398:THR:HG22 | 1:D:399:VAL:N    | 2.07                     | 0.68              |
| 2:I:52:ASP:CA    | 2:I:55:THR:HG23  | 2.24                     | 0.68              |
| 2:J:56:LEU:HD13  | 2:J:95:LEU:HG    | 1.75                     | 0.68              |
| 2:N:131:LEU:HD11 | 2:N:135:ARG:HE   | 1.59                     | 0.68              |
| 2:I:38:TYR:CE1   | 2:I:69:GLY:HA3   | 2.27                     | 0.68              |
| 1:S:344:ILE:HG23 | 3:S:456:ATP:C2   | 2.29                     | 0.68              |
| 1:U:439:LEU:H    | 1:U:439:LEU:HD23 | 1.59                     | 0.68              |
| 1:E:337:SER:HB3  | 1:E:340:ASP:OD2  | 1.94                     | 0.68              |
| 1:A:415:ASN:OD1  | 1:A:416:GLY:N    | 2.26                     | 0.68              |
| 2:I:79:ALA:HB1   | 2:I:83:ARG:HH21  | 1.58                     | 0.68              |
| 1:S:23:ALA:HA    | 1:S:331:VAL:HG21 | 1.76                     | 0.68              |
| 1:D:37:ARG:HA    | 1:D:40:LEU:HD12  | 1.76                     | 0.68              |
| 1:E:344:ILE:CG2  | 3:E:454:ATP:C2   | 2.77                     | 0.68              |
| 2:N:7:ARG:NE     | 2:N:119:GLN:HE21 | 1.91                     | 0.68              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:442:PHE:O    | 1:S:443:ILE:HD13 | 1.93                     | 0.68              |
| 1:S:370:THR:HG22 | 1:S:421:ILE:O    | 1.94                     | 0.68              |
| 2:K:137:LEU:HD11 | 2:Q:136:ALA:HB1  | 1.76                     | 0.68              |
| 2:O:131:LEU:HD11 | 2:O:135:ARG:HE   | 1.58                     | 0.68              |
| 1:V:385:ASN:HD21 | 1:V:395:ARG:HE   | 1.42                     | 0.68              |
| 1:E:20:GLN:HA    | 1:E:20:GLN:NE2   | 2.07                     | 0.67              |
| 2:G:88:LEU:O     | 2:G:88:LEU:HD23  | 1.94                     | 0.67              |
| 1:C:349:HIS:O    | 1:C:350:ALA:HB3  | 1.93                     | 0.67              |
| 1:T:42:GLU:HB3   | 1:T:43:PRO:HD3   | 1.76                     | 0.67              |
| 1:F:406:LYS:N    | 1:F:406:LYS:HD2  | 2.05                     | 0.67              |
| 1:B:405:ASP:HB3  | 1:B:406:LYS:HD2  | 1.76                     | 0.67              |
| 1:U:437:GLU:HG3  | 1:U:440:SER:HB2  | 1.76                     | 0.67              |
| 1:T:227:ILE:HG23 | 1:T:228:ASP:H    | 1.59                     | 0.67              |
| 2:L:105:ILE:CG2  | 2:L:113:VAL:HB   | 2.24                     | 0.67              |
| 1:W:42:GLU:HB3   | 1:W:43:PRO:HD3   | 1.77                     | 0.67              |
| 1:C:275:ARG:C    | 1:C:277:GLY:H    | 1.98                     | 0.67              |
| 1:A:41:GLN:HA    | 1:A:41:GLN:NE2   | 2.09                     | 0.67              |
| 1:X:37:ARG:HH21  | 1:X:302:HIS:CE1  | 2.11                     | 0.67              |
| 1:X:344:ILE:HG23 | 3:X:461:ATP:H2   | 1.59                     | 0.67              |
| 2:P:60:PHE:CE2   | 2:P:97:VAL:HG11  | 2.29                     | 0.67              |
| 1:A:79:ILE:HG22  | 1:A:103:LEU:HD13 | 1.74                     | 0.67              |
| 1:F:367:ILE:HD11 | 1:F:421:ILE:HD11 | 1.75                     | 0.67              |
| 2:L:137:LEU:CD1  | 2:R:136:ALA:HB1  | 2.24                     | 0.67              |
| 1:D:275:ARG:C    | 1:D:277:GLY:N    | 2.48                     | 0.67              |
| 1:S:5:THR:O      | 1:S:9:ILE:HG13   | 1.94                     | 0.67              |
| 1:F:5:THR:H      | 1:F:8:GLU:HB3    | 1.58                     | 0.67              |
| 1:V:370:THR:HG22 | 1:V:421:ILE:O    | 1.95                     | 0.67              |
| 1:E:52:ASN:ND2   | 1:E:305:PHE:N    | 2.41                     | 0.67              |
| 2:G:1:THR:HG23   | 2:G:33:LYS:NZ    | 2.09                     | 0.67              |
| 2:I:46:PHE:HB3   | 2:I:95:LEU:CD2   | 2.25                     | 0.67              |
| 1:B:57:GLY:O     | 1:B:310:ALA:HA   | 1.94                     | 0.67              |
| 1:X:63:LYS:NZ    | 1:X:308:SER:HB2  | 2.10                     | 0.67              |
| 1:A:37:ARG:HA    | 1:A:40:LEU:HD12  | 1.76                     | 0.67              |
| 2:K:105:ILE:HG23 | 2:K:113:VAL:HB   | 1.76                     | 0.67              |
| 1:E:23:ALA:HA    | 1:E:331:VAL:HG21 | 1.76                     | 0.67              |
| 1:T:17:ILE:HD11  | 1:T:65:GLU:HB3   | 1.76                     | 0.67              |
| 1:F:250:GLN:HA   | 1:F:250:GLN:NE2  | 2.10                     | 0.67              |
| 2:L:103:SER:O    | 2:L:104:LEU:HD12 | 1.95                     | 0.67              |
| 1:D:57:GLY:O     | 1:D:310:ALA:HA   | 1.94                     | 0.67              |
| 1:V:347:GLU:HB2  | 1:V:348:PRO:HD3  | 1.76                     | 0.67              |
| 1:C:414:MET:O    | 1:C:414:MET:HG2  | 1.94                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:279:GLN:NE2  | 1:W:320:ILE:N    | 2.41                     | 0.66              |
| 2:J:144:SER:HB3  | 2:J:147:GLU:CG   | 2.25                     | 0.66              |
| 2:M:164:ASN:ND2  | 2:M:164:ASN:H    | 1.93                     | 0.66              |
| 1:D:250:GLN:HA   | 1:D:250:GLN:NE2  | 2.09                     | 0.66              |
| 2:H:7:ARG:CD     | 2:H:119:GLN:OE1  | 2.43                     | 0.66              |
| 2:K:91:LEU:O     | 2:K:108:GLY:HA3  | 1.95                     | 0.66              |
| 2:G:107:THR:OG1  | 2:G:111:ASP:OD2  | 2.10                     | 0.66              |
| 1:E:41:GLN:HA    | 1:E:41:GLN:NE2   | 2.09                     | 0.66              |
| 1:A:264:LYS:NZ   | 1:A:279:GLN:NE2  | 2.31                     | 0.66              |
| 1:S:279:GLN:NE2  | 1:S:320:ILE:N    | 2.36                     | 0.66              |
| 2:K:55:THR:O     | 2:K:59:LEU:HD13  | 1.95                     | 0.66              |
| 1:W:247:ALA:O    | 1:W:251:ASN:N    | 2.28                     | 0.66              |
| 1:X:347:GLU:HB2  | 1:X:348:PRO:HD3  | 1.77                     | 0.66              |
| 2:M:137:LEU:O    | 2:M:141:THR:HG22 | 1.95                     | 0.66              |
| 2:O:105:ILE:HG23 | 2:O:113:VAL:HB   | 1.78                     | 0.66              |
| 1:F:63:LYS:HB2   | 3:F:455:ATP:O2B  | 1.94                     | 0.66              |
| 1:X:344:ILE:HG23 | 3:X:461:ATP:C2   | 2.30                     | 0.66              |
| 1:D:421:ILE:HG23 | 1:D:425:TYR:CD1  | 2.30                     | 0.66              |
| 1:U:65:GLU:HG2   | 3:U:458:ATP:C5'  | 2.22                     | 0.66              |
| 1:T:257:ASP:HA   | 1:T:308:SER:OG   | 1.95                     | 0.66              |
| 2:K:13:VAL:HG22  | 2:K:171:GLU:HB3  | 1.78                     | 0.66              |
| 1:U:42:GLU:HB3   | 1:U:43:PRO:HD3   | 1.75                     | 0.66              |
| 2:P:105:ILE:HG23 | 2:P:113:VAL:HB   | 1.77                     | 0.66              |
| 2:Q:60:PHE:CE2   | 2:Q:97:VAL:HG11  | 2.31                     | 0.66              |
| 1:B:256:ILE:HG21 | 1:B:259:ILE:HD12 | 1.77                     | 0.66              |
| 1:C:264:LYS:NZ   | 1:C:279:GLN:NE2  | 2.40                     | 0.66              |
| 1:E:283:LEU:HB2  | 1:E:284:PRO:HD3  | 1.77                     | 0.66              |
| 1:A:377:ILE:O    | 1:A:380:ALA:HB3  | 1.95                     | 0.66              |
| 2:I:13:VAL:HG22  | 2:I:171:GLU:HB3  | 1.77                     | 0.66              |
| 1:V:64:THR:HB    | 3:V:459:ATP:O2A  | 1.96                     | 0.66              |
| 2:L:105:ILE:HG23 | 2:L:113:VAL:HB   | 1.78                     | 0.66              |
| 1:F:52:ASN:O     | 1:F:328:PRO:HD2  | 1.96                     | 0.66              |
| 2:G:84:THR:HG22  | 2:G:85:ASP:H     | 1.60                     | 0.66              |
| 1:B:403:LEU:HD23 | 1:B:403:LEU:C    | 2.15                     | 0.66              |
| 2:M:105:ILE:HG23 | 2:M:113:VAL:HB   | 1.77                     | 0.66              |
| 2:Q:105:ILE:HG23 | 2:Q:113:VAL:HB   | 1.77                     | 0.66              |
| 1:C:435:GLU:CG   | 1:C:436:ASN:H    | 2.07                     | 0.66              |
| 1:B:83:ALA:HB1   | 1:B:262:ILE:HD13 | 1.78                     | 0.66              |
| 1:S:344:ILE:HG23 | 3:S:456:ATP:H2   | 1.60                     | 0.66              |
| 2:J:118:ASP:O    | 2:J:119:GLN:C    | 2.33                     | 0.66              |
| 1:A:20:GLN:HE21  | 1:A:20:GLN:N     | 1.94                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:415:ASN:OD1  | 1:F:416:GLY:N    | 2.29                     | 0.66              |
| 2:I:165:THR:HA   | 2:I:167:PHE:CE2  | 2.31                     | 0.66              |
| 2:M:103:SER:O    | 2:M:104:LEU:HD23 | 1.95                     | 0.66              |
| 1:S:320:ILE:HD11 | 1:S:323:LEU:HD13 | 1.77                     | 0.66              |
| 2:K:137:LEU:CD1  | 2:Q:136:ALA:HB1  | 2.25                     | 0.66              |
| 2:G:137:LEU:HD11 | 2:M:136:ALA:HB1  | 1.78                     | 0.66              |
| 2:K:46:PHE:HB3   | 2:K:95:LEU:CD2   | 2.26                     | 0.66              |
| 2:M:83:ARG:CB    | 2:R:55:THR:HG22  | 2.25                     | 0.66              |
| 1:A:23:ALA:HA    | 1:A:331:VAL:HG21 | 1.78                     | 0.65              |
| 1:C:366:ASN:HB3  | 1:C:418:THR:HG22 | 1.78                     | 0.65              |
| 2:R:137:LEU:O    | 2:R:141:THR:HG22 | 1.96                     | 0.65              |
| 1:V:42:GLU:HB3   | 1:V:43:PRO:HD3   | 1.77                     | 0.65              |
| 1:S:42:GLU:HB3   | 1:S:43:PRO:HD3   | 1.78                     | 0.65              |
| 2:I:56:LEU:HD13  | 2:I:95:LEU:HG    | 1.78                     | 0.65              |
| 1:B:443:ILE:HD11 | 2:H:72:LEU:HD11  | 1.77                     | 0.65              |
| 2:N:56:LEU:HD23  | 2:N:95:LEU:HD22  | 1.78                     | 0.65              |
| 1:F:37:ARG:HA    | 1:F:40:LEU:HD12  | 1.78                     | 0.65              |
| 2:L:1:THR:HG22   | 2:L:2:THR:N      | 2.11                     | 0.65              |
| 1:T:37:ARG:HH21  | 1:T:302:HIS:CE1  | 2.13                     | 0.65              |
| 2:L:13:VAL:HG22  | 2:L:171:GLU:HB3  | 1.79                     | 0.65              |
| 2:N:60:PHE:CE2   | 2:N:97:VAL:HG11  | 2.32                     | 0.65              |
| 1:C:415:ASN:OD1  | 1:C:416:GLY:N    | 2.28                     | 0.65              |
| 1:U:345:LEU:HD23 | 1:U:374:VAL:HG13 | 1.79                     | 0.65              |
| 1:F:280:ARG:HG3  | 1:F:280:ARG:HH11 | 1.61                     | 0.65              |
| 2:O:55:THR:HG22  | 2:P:83:ARG:CB    | 2.26                     | 0.65              |
| 1:S:347:GLU:HB2  | 1:S:348:PRO:HD3  | 1.76                     | 0.65              |
| 2:O:137:LEU:O    | 2:O:141:THR:HG22 | 1.96                     | 0.65              |
| 1:E:100:ILE:HB   | 1:E:291:VAL:HG21 | 1.76                     | 0.65              |
| 1:W:326:ARG:NH1  | 1:W:326:ARG:HB3  | 2.11                     | 0.65              |
| 1:F:352:LEU:HD13 | 1:F:400:MET:HG3  | 1.78                     | 0.65              |
| 1:F:27:VAL:HB    | 1:F:70:LEU:HD22  | 1.78                     | 0.65              |
| 1:A:283:LEU:HB2  | 1:A:284:PRO:HD3  | 1.78                     | 0.65              |
| 1:A:235:ILE:HG22 | 1:A:237:PRO:CD   | 2.26                     | 0.65              |
| 1:V:439:LEU:O    | 1:V:441:ARG:N    | 2.30                     | 0.65              |
| 2:I:137:LEU:CD1  | 2:O:136:ALA:HB1  | 2.27                     | 0.65              |
| 1:B:37:ARG:HA    | 1:B:40:LEU:CD1   | 2.26                     | 0.65              |
| 2:R:60:PHE:CE2   | 2:R:97:VAL:HG11  | 2.31                     | 0.65              |
| 1:W:257:ASP:HA   | 1:W:308:SER:OG   | 1.96                     | 0.65              |
| 1:C:52:ASN:HD22  | 1:C:305:PHE:N    | 1.95                     | 0.65              |
| 1:T:63:LYS:NZ    | 1:T:308:SER:HB2  | 2.12                     | 0.65              |
| 1:V:326:ARG:NH1  | 1:V:326:ARG:HB3  | 2.10                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:20:GLN:HE21  | 1:A:20:GLN:H     | 1.43                     | 0.65              |
| 1:C:352:LEU:HD13 | 1:C:400:MET:HG3  | 1.77                     | 0.65              |
| 1:S:18:ILE:HD11  | 1:S:343:ARG:NH2  | 2.12                     | 0.65              |
| 2:J:87:ALA:O     | 2:J:88:LEU:HB2   | 1.97                     | 0.65              |
| 1:V:36:ARG:HA    | 1:V:36:ARG:HE    | 1.62                     | 0.65              |
| 1:S:439:LEU:HG   | 1:S:440:SER:H    | 1.61                     | 0.64              |
| 1:W:63:LYS:HZ2   | 1:W:308:SER:HB2  | 1.62                     | 0.64              |
| 1:U:63:LYS:NZ    | 1:U:308:SER:HB2  | 2.12                     | 0.64              |
| 1:D:241:LYS:O    | 1:D:245:ILE:HG13 | 1.98                     | 0.64              |
| 1:U:5:THR:O      | 1:U:9:ILE:HG13   | 1.97                     | 0.64              |
| 1:D:367:ILE:CD1  | 1:D:421:ILE:HD11 | 2.27                     | 0.64              |
| 1:V:439:LEU:HG   | 1:V:440:SER:H    | 1.62                     | 0.64              |
| 2:K:107:THR:OG1  | 2:K:111:ASP:OD2  | 2.09                     | 0.64              |
| 1:T:439:LEU:HG   | 1:T:440:SER:H    | 1.60                     | 0.64              |
| 2:J:52:ASP:HA    | 2:J:55:THR:CG2   | 2.25                     | 0.64              |
| 1:B:406:LYS:HD2  | 1:B:406:LYS:N    | 2.06                     | 0.64              |
| 2:H:37:LEU:HB2   | 2:H:42:VAL:HG23  | 1.80                     | 0.64              |
| 1:F:437:GLU:O    | 1:F:438:ASP:O    | 2.14                     | 0.64              |
| 1:S:105:ASP:HB3  | 1:X:297:MET:HE2  | 1.78                     | 0.64              |
| 2:J:38:TYR:CE1   | 2:J:69:GLY:HA3   | 2.32                     | 0.64              |
| 1:S:280:ARG:HH22 | 1:T:261:LYS:HE3  | 1.61                     | 0.64              |
| 1:F:377:ILE:O    | 1:F:380:ALA:HB3  | 1.97                     | 0.64              |
| 1:W:63:LYS:NZ    | 1:W:308:SER:HB2  | 2.13                     | 0.64              |
| 2:Q:55:THR:HG22  | 2:R:83:ARG:HG2   | 1.80                     | 0.64              |
| 2:G:105:ILE:HG22 | 2:G:113:VAL:O    | 1.98                     | 0.64              |
| 1:F:20:GLN:NE2   | 1:F:20:GLN:HA    | 2.13                     | 0.64              |
| 1:X:5:THR:O      | 1:X:9:ILE:HG13   | 1.97                     | 0.64              |
| 1:S:385:ASN:HD21 | 1:S:395:ARG:HE   | 1.44                     | 0.64              |
| 1:S:36:ARG:HE    | 1:S:36:ARG:HA    | 1.61                     | 0.64              |
| 1:U:279:GLN:NE2  | 1:U:320:ILE:N    | 2.40                     | 0.64              |
| 1:X:279:GLN:NE2  | 1:X:320:ILE:N    | 2.41                     | 0.64              |
| 1:W:370:THR:HG22 | 1:W:421:ILE:O    | 1.97                     | 0.64              |
| 1:U:370:THR:HG22 | 1:U:421:ILE:O    | 1.97                     | 0.64              |
| 1:A:421:ILE:HA   | 1:A:425:TYR:HD1  | 1.63                     | 0.64              |
| 1:T:320:ILE:HD11 | 1:T:323:LEU:HD13 | 1.79                     | 0.64              |
| 1:U:344:ILE:HG23 | 3:U:458:ATP:H2   | 1.62                     | 0.64              |
| 1:E:244:ALA:O    | 1:E:247:ALA:HB3  | 1.97                     | 0.64              |
| 1:C:37:ARG:HH12  | 1:C:38:MET:HE2   | 1.63                     | 0.64              |
| 1:S:12:GLU:HG2   | 1:S:73:LEU:HD23  | 1.79                     | 0.64              |
| 1:X:245:ILE:HG22 | 1:X:249:GLU:HG3  | 1.80                     | 0.64              |
| 1:C:27:VAL:HB    | 1:C:70:LEU:HD22  | 1.78                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:112:ARG:HA   | 1:B:240:LEU:HD21 | 1.80                     | 0.64              |
| 1:S:17:ILE:HD11  | 1:S:65:GLU:HB3   | 1.79                     | 0.64              |
| 2:H:55:THR:O     | 2:H:59:LEU:HD13  | 1.97                     | 0.64              |
| 1:V:257:ASP:HA   | 1:V:308:SER:OG   | 1.98                     | 0.64              |
| 1:X:442:PHE:N    | 1:X:442:PHE:HD1  | 1.87                     | 0.64              |
| 1:A:57:GLY:HA3   | 1:A:63:LYS:HE3   | 1.80                     | 0.64              |
| 2:J:17:ASP:O     | 2:J:33:LYS:HD2   | 1.98                     | 0.64              |
| 1:W:36:ARG:HE    | 1:W:36:ARG:HA    | 1.62                     | 0.64              |
| 1:U:257:ASP:HA   | 1:U:308:SER:OG   | 1.98                     | 0.64              |
| 1:U:36:ARG:HA    | 1:U:36:ARG:HE    | 1.61                     | 0.64              |
| 1:W:320:ILE:HD11 | 1:W:323:LEU:HD13 | 1.80                     | 0.63              |
| 2:Q:56:LEU:HD23  | 2:Q:95:LEU:HD22  | 1.80                     | 0.63              |
| 1:S:257:ASP:HA   | 1:S:308:SER:OG   | 1.97                     | 0.63              |
| 2:G:80:LYS:HA    | 2:G:83:ARG:HD3   | 1.80                     | 0.63              |
| 1:B:421:ILE:HG23 | 1:B:425:TYR:HD1  | 1.59                     | 0.63              |
| 1:X:17:ILE:HD13  | 1:X:66:ILE:CG1   | 2.28                     | 0.63              |
| 1:A:37:ARG:HH22  | 1:A:250:GLN:HE22 | 1.47                     | 0.63              |
| 2:O:76:VAL:HG22  | 1:U:443:ILE:HD11 | 1.78                     | 0.63              |
| 1:D:369:PHE:CE2  | 1:D:421:ILE:HD12 | 2.33                     | 0.63              |
| 1:C:283:LEU:HB2  | 1:C:284:PRO:HD3  | 1.80                     | 0.63              |
| 1:D:100:ILE:HB   | 1:D:291:VAL:HG21 | 1.79                     | 0.63              |
| 1:B:347:GLU:HB2  | 1:B:348:PRO:HD3  | 1.80                     | 0.63              |
| 2:R:105:ILE:HG23 | 2:R:113:VAL:HB   | 1.80                     | 0.63              |
| 1:T:326:ARG:HB3  | 1:T:326:ARG:NH1  | 2.13                     | 0.63              |
| 1:V:441:ARG:HB3  | 1:V:442:PHE:CD1  | 2.33                     | 0.63              |
| 1:B:20:GLN:NE2   | 1:B:20:GLN:HA    | 2.11                     | 0.63              |
| 2:H:91:LEU:N     | 2:H:91:LEU:HD12  | 2.13                     | 0.63              |
| 2:K:86:ARG:HG2   | 2:K:87:ALA:N     | 2.13                     | 0.63              |
| 1:V:23:ALA:O     | 1:V:27:VAL:HG23  | 1.99                     | 0.63              |
| 2:K:13:VAL:HG22  | 2:K:171:GLU:CB   | 2.28                     | 0.63              |
| 1:C:391:ILE:HG22 | 1:D:321:PRO:HB3  | 1.80                     | 0.63              |
| 1:S:441:ARG:HB3  | 1:S:442:PHE:CD1  | 2.29                     | 0.63              |
| 1:T:370:THR:HG22 | 1:T:421:ILE:O    | 1.98                     | 0.63              |
| 1:B:351:SER:O    | 1:B:355:GLN:HG3  | 1.98                     | 0.63              |
| 1:U:326:ARG:HB3  | 1:U:326:ARG:NH1  | 2.13                     | 0.63              |
| 1:T:345:LEU:HD23 | 1:T:374:VAL:HG13 | 1.80                     | 0.63              |
| 1:U:17:ILE:HD11  | 1:U:65:GLU:HB3   | 1.80                     | 0.63              |
| 2:Q:164:ASN:ND2  | 2:Q:164:ASN:H    | 1.95                     | 0.63              |
| 1:X:370:THR:HG22 | 1:X:421:ILE:O    | 1.98                     | 0.63              |
| 1:A:36:ARG:O     | 1:A:39:GLN:HB3   | 1.98                     | 0.63              |
| 1:F:56:ILE:N     | 1:F:56:ILE:HD12  | 2.13                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:437:GLU:HG3  | 1:T:438:ASP:N    | 2.08                     | 0.63              |
| 2:P:56:LEU:HD23  | 2:P:95:LEU:HD22  | 1.81                     | 0.63              |
| 1:X:36:ARG:HE    | 1:X:36:ARG:HA    | 1.63                     | 0.63              |
| 1:T:385:ASN:HD21 | 1:T:395:ARG:HE   | 1.47                     | 0.63              |
| 1:E:433:VAL:O    | 1:E:433:VAL:HG13 | 1.98                     | 0.63              |
| 1:S:27:VAL:HG21  | 1:S:66:ILE:HG21  | 1.81                     | 0.63              |
| 1:B:104:THR:HA   | 1:B:248:VAL:CG2  | 2.28                     | 0.63              |
| 1:E:414:MET:HG2  | 1:E:414:MET:O    | 1.99                     | 0.63              |
| 1:V:63:LYS:NZ    | 1:V:308:SER:HB2  | 2.13                     | 0.63              |
| 1:C:57:GLY:HA3   | 1:C:63:LYS:HE3   | 1.81                     | 0.63              |
| 2:K:165:THR:HA   | 2:K:167:PHE:CE2  | 2.34                     | 0.63              |
| 1:E:264:LYS:CE   | 1:E:279:GLN:HE22 | 2.11                     | 0.63              |
| 1:W:17:ILE:HD11  | 1:W:65:GLU:HB3   | 1.79                     | 0.63              |
| 1:E:20:GLN:NE2   | 1:E:20:GLN:CA    | 2.58                     | 0.63              |
| 1:E:20:GLN:N     | 1:E:20:GLN:HE21  | 1.95                     | 0.63              |
| 1:X:236:ASN:H    | 1:X:237:PRO:HD3  | 1.63                     | 0.63              |
| 2:G:120:ILE:HD11 | 2:G:138:VAL:HG21 | 1.80                     | 0.63              |
| 1:A:352:LEU:HD13 | 1:A:400:MET:HG3  | 1.80                     | 0.63              |
| 1:F:421:ILE:HG23 | 1:F:425:TYR:CD1  | 2.34                     | 0.63              |
| 1:E:60:GLY:HA2   | 3:E:454:ATP:O3A  | 1.99                     | 0.63              |
| 1:X:385:ASN:HD21 | 1:X:395:ARG:HE   | 1.46                     | 0.63              |
| 2:I:37:LEU:HB2   | 2:I:42:VAL:CG2   | 2.29                     | 0.63              |
| 1:E:5:THR:O      | 1:E:9:ILE:HG13   | 1.99                     | 0.63              |
| 1:X:286:VAL:HA   | 1:X:305:PHE:CE1  | 2.34                     | 0.63              |
| 2:M:7:ARG:NE     | 2:M:119:GLN:OE1  | 2.32                     | 0.62              |
| 1:S:439:LEU:O    | 1:S:441:ARG:N    | 2.32                     | 0.62              |
| 1:U:63:LYS:HZ2   | 1:U:308:SER:HB2  | 1.63                     | 0.62              |
| 1:E:36:ARG:O     | 1:E:39:GLN:HB3   | 1.99                     | 0.62              |
| 2:H:42:VAL:HG12  | 2:H:99:ASP:HB3   | 1.80                     | 0.62              |
| 2:H:17:ASP:O     | 2:H:33:LYS:HD2   | 1.98                     | 0.62              |
| 1:X:18:ILE:HD11  | 1:X:343:ARG:NH2  | 2.14                     | 0.62              |
| 1:W:37:ARG:HH11  | 1:W:37:ARG:HG2   | 1.64                     | 0.62              |
| 1:F:20:GLN:HA    | 1:F:20:GLN:HE21  | 1.63                     | 0.62              |
| 1:A:367:ILE:CD1  | 1:A:421:ILE:HD11 | 2.28                     | 0.62              |
| 1:X:326:ARG:NH1  | 1:X:326:ARG:HB3  | 2.13                     | 0.62              |
| 2:J:13:VAL:HG22  | 2:J:171:GLU:HB3  | 1.79                     | 0.62              |
| 1:D:362:THR:CG2  | 1:E:39:GLN:HG2   | 2.28                     | 0.62              |
| 1:E:403:LEU:C    | 1:E:403:LEU:HD23 | 2.19                     | 0.62              |
| 2:L:37:LEU:HB2   | 2:L:42:VAL:CG2   | 2.28                     | 0.62              |
| 1:S:63:LYS:HZ2   | 1:S:63:LYS:HB2   | 1.64                     | 0.62              |
| 1:C:362:THR:CG2  | 1:D:39:GLN:HG2   | 2.28                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:439:LEU:O    | 1:F:440:SER:C    | 2.36                     | 0.62              |
| 1:A:112:ARG:O    | 1:A:114:GLN:N    | 2.26                     | 0.62              |
| 1:W:27:VAL:HG21  | 1:W:66:ILE:HG21  | 1.81                     | 0.62              |
| 2:Q:105:ILE:CG2  | 2:Q:113:VAL:HB   | 2.29                     | 0.62              |
| 2:M:118:ASP:C    | 2:M:118:ASP:OD1  | 2.36                     | 0.62              |
| 1:W:385:ASN:HD21 | 1:W:395:ARG:HE   | 1.45                     | 0.62              |
| 1:C:20:GLN:HE21  | 1:C:20:GLN:CA    | 2.12                     | 0.62              |
| 1:B:58:PRO:O     | 1:B:63:LYS:NZ    | 2.32                     | 0.62              |
| 2:N:8:ARG:CB     | 2:N:8:ARG:HH11   | 2.12                     | 0.62              |
| 1:W:326:ARG:HH11 | 1:W:326:ARG:CB   | 2.13                     | 0.62              |
| 2:K:5:SER:HB2    | 2:K:14:VAL:HG22  | 1.81                     | 0.62              |
| 1:C:356:TYR:HE1  | 1:C:400:MET:HB3  | 1.64                     | 0.62              |
| 1:D:337:SER:HB3  | 1:D:340:ASP:OD2  | 1.98                     | 0.62              |
| 1:X:320:ILE:HD11 | 1:X:323:LEU:HD13 | 1.82                     | 0.62              |
| 1:T:12:GLU:HG2   | 1:T:73:LEU:HD23  | 1.82                     | 0.62              |
| 1:W:64:THR:HB    | 3:W:460:ATP:O2A  | 2.00                     | 0.62              |
| 1:A:233:LYS:NZ   | 1:A:234:LEU:HB2  | 2.15                     | 0.62              |
| 2:N:3:ILE:O      | 2:N:122:ALA:HA   | 1.99                     | 0.62              |
| 2:J:52:ASP:OD2   | 2:J:91:LEU:HA    | 2.00                     | 0.62              |
| 1:C:405:ASP:HB3  | 1:C:406:LYS:HD2  | 1.80                     | 0.62              |
| 1:S:63:LYS:NZ    | 1:S:308:SER:HB2  | 2.15                     | 0.62              |
| 2:P:164:ASN:ND2  | 2:P:164:ASN:H    | 1.96                     | 0.62              |
| 1:V:27:VAL:HG21  | 1:V:66:ILE:HG21  | 1.82                     | 0.62              |
| 1:D:322:GLU:N    | 1:D:322:GLU:OE2  | 2.29                     | 0.62              |
| 2:H:107:THR:OG1  | 2:H:111:ASP:OD2  | 2.11                     | 0.62              |
| 2:N:105:ILE:CG2  | 2:N:113:VAL:HB   | 2.30                     | 0.62              |
| 2:H:137:LEU:CD1  | 2:N:136:ALA:HB1  | 2.30                     | 0.62              |
| 1:F:38:MET:HG3   | 1:F:45:ARG:HH12  | 1.65                     | 0.62              |
| 2:K:1:THR:HG23   | 2:K:33:LYS:HD3   | 1.82                     | 0.62              |
| 1:D:407:ILE:HD11 | 1:D:419:VAL:HG11 | 1.82                     | 0.62              |
| 1:V:12:GLU:HG2   | 1:V:73:LEU:HD23  | 1.81                     | 0.62              |
| 1:F:264:LYS:HE3  | 1:F:264:LYS:H    | 1.64                     | 0.62              |
| 1:U:17:ILE:HD13  | 1:U:66:ILE:CG1   | 2.30                     | 0.62              |
| 2:M:105:ILE:CG2  | 2:M:113:VAL:HB   | 2.29                     | 0.62              |
| 2:O:56:LEU:HD23  | 2:O:95:LEU:HD22  | 1.82                     | 0.62              |
| 1:T:247:ALA:O    | 1:T:251:ASN:HB2  | 2.00                     | 0.62              |
| 1:T:36:ARG:HE    | 1:T:36:ARG:HA    | 1.63                     | 0.62              |
| 2:I:52:ASP:HA    | 2:I:55:THR:CG2   | 2.29                     | 0.61              |
| 1:E:403:LEU:CD2  | 1:E:404:MET:SD   | 2.88                     | 0.61              |
| 2:H:46:PHE:HB3   | 2:H:95:LEU:CD2   | 2.30                     | 0.61              |
| 2:R:8:ARG:CB     | 2:R:8:ARG:HH11   | 2.13                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:421:ILE:HA   | 1:C:425:TYR:HD1  | 1.63                     | 0.61              |
| 1:X:112:ARG:HB2  | 1:X:240:LEU:HD21 | 1.81                     | 0.61              |
| 1:W:345:LEU:HD23 | 1:W:374:VAL:HG13 | 1.80                     | 0.61              |
| 2:M:7:ARG:HH21   | 2:M:103:SER:HB3  | 1.64                     | 0.61              |
| 1:F:381:ALA:O    | 1:F:384:VAL:HG13 | 2.00                     | 0.61              |
| 1:D:405:ASP:HB3  | 1:D:406:LYS:HD2  | 1.81                     | 0.61              |
| 2:R:164:ASN:H    | 2:R:164:ASN:ND2  | 1.98                     | 0.61              |
| 1:A:232:ALA:HA   | 1:A:235:ILE:HD12 | 1.81                     | 0.61              |
| 2:M:55:THR:HG22  | 2:N:83:ARG:CG    | 2.28                     | 0.61              |
| 1:F:20:GLN:NE2   | 1:F:20:GLN:CA    | 2.63                     | 0.61              |
| 1:S:326:ARG:NH1  | 1:S:326:ARG:HB3  | 2.14                     | 0.61              |
| 1:C:367:ILE:HD11 | 1:C:421:ILE:CD1  | 2.30                     | 0.61              |
| 1:A:60:GLY:HA2   | 3:A:450:ATP:O3A  | 2.00                     | 0.61              |
| 1:B:13:LEU:HD13  | 1:B:24:LYS:HG2   | 1.82                     | 0.61              |
| 1:D:391:ILE:HG22 | 1:E:321:PRO:HB3  | 1.82                     | 0.61              |
| 2:M:17:ASP:HB2   | 2:M:164:ASN:HD22 | 1.66                     | 0.61              |
| 2:Q:17:ASP:HB2   | 2:Q:164:ASN:HD21 | 1.64                     | 0.61              |
| 1:S:398:THR:HA   | 1:X:328:PRO:HB3  | 1.81                     | 0.61              |
| 1:F:20:GLN:N     | 1:F:20:GLN:HE21  | 1.98                     | 0.61              |
| 1:F:4:MET:HE2    | 1:F:9:ILE:HA     | 1.81                     | 0.61              |
| 1:W:280:ARG:HH22 | 1:X:261:LYS:HE3  | 1.64                     | 0.61              |
| 1:T:120:ARG:NH2  | 1:T:121:ALA:HB2  | 2.16                     | 0.61              |
| 2:Q:7:ARG:HH21   | 2:Q:103:SER:HB3  | 1.65                     | 0.61              |
| 2:Q:72:LEU:O     | 2:Q:76:VAL:HG23  | 2.01                     | 0.61              |
| 2:G:17:ASP:OD2   | 2:G:33:LYS:HE3   | 2.00                     | 0.61              |
| 2:O:8:ARG:CB     | 2:O:8:ARG:HH11   | 2.12                     | 0.61              |
| 1:D:79:ILE:CG2   | 1:D:103:LEU:HD13 | 2.31                     | 0.61              |
| 1:C:370:THR:HG23 | 1:C:421:ILE:O    | 1.99                     | 0.61              |
| 1:D:283:LEU:HB2  | 1:D:284:PRO:HD3  | 1.82                     | 0.61              |
| 1:V:51:LYS:HE2   | 1:W:356:TYR:OH   | 2.00                     | 0.61              |
| 2:R:3:ILE:O      | 2:R:122:ALA:HA   | 2.01                     | 0.61              |
| 1:C:237:PRO:HB3  | 1:C:241:LYS:HZ1  | 1.66                     | 0.61              |
| 2:I:83:ARG:HG2   | 2:J:55:THR:CB    | 2.29                     | 0.61              |
| 2:P:105:ILE:CG2  | 2:P:113:VAL:HB   | 2.29                     | 0.61              |
| 2:P:137:LEU:O    | 2:P:141:THR:HG22 | 2.00                     | 0.61              |
| 2:J:105:ILE:HG23 | 2:J:113:VAL:HB   | 1.80                     | 0.61              |
| 1:V:326:ARG:CB   | 1:V:326:ARG:HH11 | 2.12                     | 0.61              |
| 2:I:107:THR:OG1  | 2:I:111:ASP:OD2  | 2.10                     | 0.61              |
| 1:D:264:LYS:H    | 1:D:264:LYS:HE3  | 1.63                     | 0.61              |
| 1:T:283:LEU:HD13 | 1:T:323:LEU:HD12 | 1.83                     | 0.61              |
| 1:E:367:ILE:CD1  | 1:E:421:ILE:HD11 | 2.29                     | 0.61              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:64:THR:HB    | 3:S:456:ATP:O2A  | 2.00                     | 0.61              |
| 2:M:8:ARG:CB     | 2:M:8:ARG:HH11   | 2.10                     | 0.61              |
| 2:J:42:VAL:HG12  | 2:J:99:ASP:HB3   | 1.82                     | 0.61              |
| 1:E:440:SER:O    | 1:E:442:PHE:N    | 2.34                     | 0.61              |
| 1:B:52:ASN:O     | 1:B:328:PRO:HD2  | 2.00                     | 0.61              |
| 1:B:227:ILE:HG12 | 1:B:227:ILE:O    | 1.99                     | 0.61              |
| 2:H:144:SER:HB3  | 2:H:147:GLU:CG   | 2.31                     | 0.61              |
| 1:F:57:GLY:HA3   | 1:F:63:LYS:HE3   | 1.83                     | 0.61              |
| 2:K:57:PHE:HA    | 2:K:95:LEU:HD11  | 1.82                     | 0.61              |
| 2:Q:3:ILE:O      | 2:Q:122:ALA:HA   | 2.00                     | 0.61              |
| 1:U:12:GLU:HG2   | 1:U:73:LEU:HD23  | 1.83                     | 0.61              |
| 1:F:37:ARG:HH22  | 1:F:250:GLN:HE22 | 1.48                     | 0.61              |
| 1:C:443:ILE:HG12 | 2:I:112:VAL:HG21 | 1.82                     | 0.61              |
| 1:F:351:SER:O    | 1:F:355:GLN:HG3  | 2.00                     | 0.61              |
| 1:S:15:GLN:O     | 1:S:349:HIS:N    | 2.31                     | 0.61              |
| 1:V:80:LYS:HG3   | 1:V:255:PHE:HD2  | 1.66                     | 0.61              |
| 1:X:345:LEU:HD23 | 1:X:374:VAL:HG13 | 1.82                     | 0.61              |
| 1:X:12:GLU:HG2   | 1:X:73:LEU:HD23  | 1.83                     | 0.61              |
| 1:B:370:THR:HG23 | 1:B:421:ILE:O    | 2.00                     | 0.61              |
| 1:B:362:THR:HG21 | 1:C:39:GLN:HG2   | 1.82                     | 0.61              |
| 2:K:105:ILE:HG22 | 2:K:113:VAL:O    | 2.01                     | 0.61              |
| 1:X:326:ARG:CB   | 1:X:326:ARG:HH11 | 2.14                     | 0.61              |
| 1:V:5:THR:OG1    | 1:V:6:PRO:HD2    | 2.01                     | 0.61              |
| 1:S:442:PHE:N    | 1:S:442:PHE:CD1  | 2.69                     | 0.61              |
| 1:B:264:LYS:HE3  | 1:B:264:LYS:H    | 1.64                     | 0.61              |
| 1:W:283:LEU:HD13 | 1:W:323:LEU:HD12 | 1.83                     | 0.61              |
| 1:V:37:ARG:HG2   | 1:V:37:ARG:HH11  | 1.66                     | 0.61              |
| 1:C:37:ARG:HG2   | 1:C:38:MET:N     | 2.15                     | 0.61              |
| 1:F:34:ARG:CZ    | 1:F:251:ASN:HA   | 2.31                     | 0.61              |
| 1:C:235:ILE:HG22 | 1:C:236:ASN:N    | 2.14                     | 0.61              |
| 1:F:37:ARG:HB2   | 1:F:48:VAL:HG11  | 1.83                     | 0.60              |
| 2:J:37:LEU:HD21  | 2:J:57:PHE:CZ    | 2.36                     | 0.60              |
| 1:D:104:THR:HA   | 1:D:248:VAL:CG2  | 2.31                     | 0.60              |
| 1:V:63:LYS:HZ2   | 1:V:308:SER:HB2  | 1.64                     | 0.60              |
| 1:A:407:ILE:HD11 | 1:A:419:VAL:HG11 | 1.82                     | 0.60              |
| 1:V:60:GLY:HA3   | 1:V:392:GLY:HA3  | 1.82                     | 0.60              |
| 2:H:13:VAL:HG22  | 2:H:171:GLU:HB3  | 1.82                     | 0.60              |
| 1:A:435:GLU:O    | 1:A:437:GLU:N    | 2.28                     | 0.60              |
| 2:I:17:ASP:HB2   | 2:I:164:ASN:HD22 | 1.63                     | 0.60              |
| 1:S:362:THR:HG21 | 1:X:39:GLN:HB2   | 1.83                     | 0.60              |
| 2:O:55:THR:HG22  | 2:P:83:ARG:HG2   | 1.83                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:60:PHE:CE2   | 2:M:97:VAL:HG11  | 2.37                     | 0.60              |
| 1:A:443:ILE:HD11 | 2:G:72:LEU:HD11  | 1.83                     | 0.60              |
| 1:D:250:GLN:HE21 | 1:D:250:GLN:HA   | 1.65                     | 0.60              |
| 1:S:37:ARG:HH11  | 1:S:37:ARG:HG2   | 1.66                     | 0.60              |
| 1:V:20:GLN:O     | 1:V:21:ALA:HB2   | 2.01                     | 0.60              |
| 1:E:25:ARG:O     | 1:E:28:ALA:HB3   | 2.02                     | 0.60              |
| 1:D:12:GLU:O     | 1:D:15:GLN:HB2   | 2.01                     | 0.60              |
| 1:W:20:GLN:O     | 1:W:21:ALA:HB2   | 2.02                     | 0.60              |
| 1:U:303:ILE:HG22 | 1:U:304:LEU:N    | 2.16                     | 0.60              |
| 1:A:443:ILE:HG12 | 2:G:112:VAL:HG21 | 1.83                     | 0.60              |
| 2:O:164:ASN:H    | 2:O:164:ASN:ND2  | 1.98                     | 0.60              |
| 1:B:275:ARG:C    | 1:B:277:GLY:N    | 2.55                     | 0.60              |
| 2:J:137:LEU:HD11 | 2:P:136:ALA:HB1  | 1.82                     | 0.60              |
| 1:C:370:THR:O    | 1:C:373:ALA:HB3  | 2.01                     | 0.60              |
| 1:F:5:THR:O      | 1:F:9:ILE:HG13   | 2.02                     | 0.60              |
| 1:S:286:VAL:HA   | 1:S:305:PHE:CE1  | 2.37                     | 0.60              |
| 1:W:386:GLU:HG2  | 1:W:386:GLU:O    | 2.00                     | 0.60              |
| 2:G:17:ASP:HB2   | 2:G:164:ASN:HD22 | 1.66                     | 0.60              |
| 1:V:434:VAL:HG12 | 1:V:435:GLU:N    | 2.15                     | 0.60              |
| 1:C:300:THR:HA   | 1:C:303:ILE:HG12 | 1.83                     | 0.60              |
| 1:B:437:GLU:O    | 1:B:438:ASP:O    | 2.18                     | 0.60              |
| 1:C:20:GLN:N     | 1:C:20:GLN:HE21  | 1.99                     | 0.60              |
| 2:R:105:ILE:CG2  | 2:R:113:VAL:HB   | 2.32                     | 0.60              |
| 2:L:42:VAL:HG12  | 2:L:99:ASP:HB3   | 1.82                     | 0.60              |
| 1:X:257:ASP:HA   | 1:X:308:SER:OG   | 2.02                     | 0.60              |
| 1:U:326:ARG:CB   | 1:U:326:ARG:HH11 | 2.15                     | 0.60              |
| 2:G:60:PHE:CE2   | 2:G:97:VAL:HG11  | 2.37                     | 0.60              |
| 1:C:57:GLY:O     | 1:C:310:ALA:HA   | 2.01                     | 0.60              |
| 1:B:415:ASN:OD1  | 1:B:416:GLY:N    | 2.34                     | 0.60              |
| 1:F:109:LYS:O    | 1:F:113:GLN:HB2  | 2.01                     | 0.60              |
| 1:A:440:SER:O    | 1:A:443:ILE:N    | 2.34                     | 0.60              |
| 2:Q:8:ARG:HH11   | 2:Q:8:ARG:CB     | 2.14                     | 0.60              |
| 1:X:17:ILE:HD11  | 1:X:65:GLU:HB3   | 1.82                     | 0.60              |
| 1:V:17:ILE:HD11  | 1:V:65:GLU:HB3   | 1.83                     | 0.60              |
| 2:M:72:LEU:O     | 2:M:76:VAL:HG23  | 2.02                     | 0.60              |
| 1:X:442:PHE:N    | 1:X:442:PHE:CD1  | 2.59                     | 0.60              |
| 1:B:338:ALA:N    | 1:B:382:PHE:HD1  | 2.00                     | 0.60              |
| 1:X:17:ILE:HD13  | 1:X:66:ILE:HG12  | 1.83                     | 0.60              |
| 1:A:41:GLN:HA    | 1:A:41:GLN:HE21  | 1.65                     | 0.60              |
| 1:E:31:LEU:HD21  | 1:E:74:ALA:HB2   | 1.82                     | 0.60              |
| 2:L:52:ASP:HA    | 2:L:55:THR:CG2   | 2.27                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:1:THR:HG22   | 2:G:2:THR:N      | 2.17                     | 0.60              |
| 1:C:56:ILE:N     | 1:C:56:ILE:HD12  | 2.16                     | 0.60              |
| 1:T:439:LEU:HD23 | 1:T:439:LEU:H    | 1.67                     | 0.60              |
| 1:U:27:VAL:HG21  | 1:U:66:ILE:HG21  | 1.84                     | 0.60              |
| 1:T:23:ALA:O     | 1:T:27:VAL:HG23  | 2.02                     | 0.60              |
| 1:F:108:MET:HG3  | 1:F:295:HIS:CE1  | 2.37                     | 0.60              |
| 2:N:112:VAL:HB   | 1:T:443:ILE:HD13 | 1.85                     | 0.59              |
| 1:F:441:ARG:NH2  | 2:G:36:ARG:O     | 2.34                     | 0.59              |
| 1:E:443:ILE:HG12 | 2:K:112:VAL:HG21 | 1.84                     | 0.59              |
| 1:S:20:GLN:O     | 1:S:21:ALA:HB2   | 2.01                     | 0.59              |
| 1:B:377:ILE:O    | 1:B:380:ALA:HB3  | 2.02                     | 0.59              |
| 1:V:300:THR:HG22 | 1:V:303:ILE:HD11 | 1.84                     | 0.59              |
| 1:E:409:PHE:CD2  | 1:F:25:ARG:CZ    | 2.84                     | 0.59              |
| 1:W:12:GLU:HG2   | 1:W:73:LEU:HD23  | 1.83                     | 0.59              |
| 1:D:52:ASN:O     | 1:D:328:PRO:HD2  | 2.01                     | 0.59              |
| 1:A:347:GLU:HB2  | 1:A:348:PRO:HD3  | 1.84                     | 0.59              |
| 1:U:283:LEU:HD13 | 1:U:323:LEU:HD12 | 1.82                     | 0.59              |
| 1:U:300:THR:HG22 | 1:U:303:ILE:HD11 | 1.84                     | 0.59              |
| 1:W:48:VAL:HA    | 1:X:355:GLN:OE1  | 2.02                     | 0.59              |
| 2:N:55:THR:HG22  | 2:O:83:ARG:HG2   | 1.83                     | 0.59              |
| 2:G:8:ARG:O      | 2:G:9:ASN:HB2    | 2.02                     | 0.59              |
| 2:H:79:ALA:HB1   | 2:H:83:ARG:HH21  | 1.66                     | 0.59              |
| 1:T:17:ILE:HD13  | 1:T:66:ILE:CG1   | 2.32                     | 0.59              |
| 1:S:27:VAL:HG21  | 1:S:66:ILE:CG2   | 2.32                     | 0.59              |
| 1:X:300:THR:HG22 | 1:X:303:ILE:HD11 | 1.82                     | 0.59              |
| 2:P:7:ARG:HH21   | 2:P:103:SER:HB3  | 1.67                     | 0.59              |
| 1:D:437:GLU:HG2  | 1:D:438:ASP:N    | 2.17                     | 0.59              |
| 1:C:330:ARG:HH11 | 1:C:330:ARG:HG3  | 1.68                     | 0.59              |
| 1:F:264:LYS:CE   | 1:F:279:GLN:HE22 | 2.14                     | 0.59              |
| 2:G:52:ASP:CA    | 2:G:55:THR:HG23  | 2.33                     | 0.59              |
| 1:T:326:ARG:HH11 | 1:T:326:ARG:CB   | 2.14                     | 0.59              |
| 1:S:326:ARG:HH11 | 1:S:326:ARG:CB   | 2.15                     | 0.59              |
| 2:H:13:VAL:HG22  | 2:H:171:GLU:CB   | 2.33                     | 0.59              |
| 2:P:89:ARG:HH11  | 2:Q:87:ALA:HB2   | 1.67                     | 0.59              |
| 1:X:283:LEU:HD13 | 1:X:323:LEU:HD12 | 1.84                     | 0.59              |
| 1:U:20:GLN:O     | 1:U:21:ALA:HB2   | 2.02                     | 0.59              |
| 1:B:234:LEU:H    | 1:B:234:LEU:HD23 | 1.68                     | 0.59              |
| 1:T:23:ALA:HA    | 1:T:331:VAL:CG2  | 2.33                     | 0.59              |
| 1:S:23:ALA:O     | 1:S:27:VAL:HG23  | 2.03                     | 0.59              |
| 2:J:13:VAL:HG22  | 2:J:171:GLU:CB   | 2.33                     | 0.59              |
| 2:N:89:ARG:HH11  | 2:O:87:ALA:HB2   | 1.67                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:3:ILE:O      | 2:P:122:ALA:HA   | 2.01                     | 0.59              |
| 1:W:442:PHE:HD1  | 1:W:442:PHE:N    | 2.01                     | 0.59              |
| 2:I:83:ARG:CG    | 2:J:55:THR:HG22  | 2.26                     | 0.59              |
| 1:V:320:ILE:HD11 | 1:V:323:LEU:HD13 | 1.85                     | 0.59              |
| 1:S:283:LEU:HD13 | 1:S:323:LEU:HD12 | 1.82                     | 0.59              |
| 1:W:23:ALA:O     | 1:W:27:VAL:HG23  | 2.01                     | 0.59              |
| 1:B:20:GLN:HE21  | 1:B:20:GLN:N     | 2.00                     | 0.59              |
| 1:F:250:GLN:HA   | 1:F:250:GLN:HE21 | 1.67                     | 0.59              |
| 2:L:83:ARG:HH21  | 2:L:111:ASP:HA   | 1.68                     | 0.59              |
| 1:W:39:GLN:HB2   | 1:X:362:THR:HG21 | 1.84                     | 0.59              |
| 2:Q:112:VAL:HB   | 1:W:443:ILE:HD13 | 1.83                     | 0.59              |
| 2:N:7:ARG:HH21   | 2:N:103:SER:HB3  | 1.66                     | 0.59              |
| 1:T:279:GLN:NE2  | 1:T:320:ILE:N    | 2.41                     | 0.59              |
| 1:E:236:ASN:ND2  | 1:E:239:GLU:HB2  | 2.18                     | 0.59              |
| 2:H:78:LEU:HD11  | 2:H:82:TRP:CZ3   | 2.38                     | 0.59              |
| 2:O:76:VAL:CG1   | 1:U:442:PHE:HD2  | 2.14                     | 0.59              |
| 1:S:15:GLN:O     | 1:S:348:PRO:HA   | 2.03                     | 0.59              |
| 1:C:58:PRO:O     | 1:C:63:LYS:NZ    | 2.30                     | 0.59              |
| 1:T:79:ILE:HG22  | 1:T:103:LEU:HD13 | 1.84                     | 0.59              |
| 1:U:286:VAL:HA   | 1:U:305:PHE:CE1  | 2.36                     | 0.59              |
| 1:W:387:LYS:HZ1  | 1:W:435:GLU:HG3  | 1.68                     | 0.59              |
| 1:U:259:ILE:O    | 1:U:262:ILE:HG12 | 2.03                     | 0.59              |
| 1:A:406:LYS:H    | 1:A:406:LYS:CD   | 2.04                     | 0.59              |
| 1:D:275:ARG:O    | 1:D:277:GLY:N    | 2.35                     | 0.59              |
| 1:X:23:ALA:O     | 1:X:27:VAL:HG23  | 2.03                     | 0.59              |
| 2:O:7:ARG:HH21   | 2:O:103:SER:HB3  | 1.68                     | 0.59              |
| 1:C:37:ARG:HH22  | 1:C:250:GLN:HE22 | 1.51                     | 0.59              |
| 1:E:391:ILE:HG22 | 1:F:321:PRO:HB3  | 1.83                     | 0.59              |
| 2:I:120:ILE:HD11 | 2:I:138:VAL:HG21 | 1.84                     | 0.59              |
| 1:S:345:LEU:HD23 | 1:S:374:VAL:HG13 | 1.84                     | 0.59              |
| 1:T:60:GLY:HA3   | 1:T:392:GLY:HA3  | 1.84                     | 0.59              |
| 1:D:360:MET:CE   | 1:D:360:MET:HA   | 2.33                     | 0.59              |
| 1:T:386:GLU:O    | 1:T:386:GLU:HG2  | 2.02                     | 0.59              |
| 2:R:37:LEU:HD23  | 1:S:441:ARG:HH22 | 1.68                     | 0.59              |
| 2:O:105:ILE:CG2  | 2:O:113:VAL:HB   | 2.32                     | 0.59              |
| 2:N:164:ASN:ND2  | 2:N:164:ASN:H    | 2.01                     | 0.59              |
| 2:H:17:ASP:OD2   | 2:H:33:LYS:HE3   | 2.03                     | 0.59              |
| 1:U:439:LEU:O    | 1:U:441:ARG:N    | 2.36                     | 0.59              |
| 2:O:89:ARG:HH11  | 2:P:87:ALA:HB2   | 1.68                     | 0.59              |
| 1:V:245:ILE:O    | 1:V:249:GLU:HG3  | 2.03                     | 0.59              |
| 1:B:56:ILE:N     | 1:B:56:ILE:HD12  | 2.18                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:230:GLU:O    | 1:B:231:ALA:CB   | 2.51                     | 0.59              |
| 2:N:56:LEU:CD2   | 2:N:95:LEU:HD22  | 2.33                     | 0.59              |
| 1:D:351:SER:O    | 1:D:355:GLN:HG3  | 2.03                     | 0.59              |
| 1:E:275:ARG:C    | 1:E:277:GLY:N    | 2.54                     | 0.59              |
| 2:I:24:ASN:O     | 2:N:161:VAL:HG13 | 2.03                     | 0.59              |
| 1:D:264:LYS:NZ   | 1:D:319:LEU:HA   | 2.18                     | 0.58              |
| 2:J:1:THR:CG2    | 2:J:33:LYS:HD3   | 2.33                     | 0.58              |
| 2:G:46:PHE:HB3   | 2:G:95:LEU:CD2   | 2.33                     | 0.58              |
| 1:X:20:GLN:O     | 1:X:21:ALA:HB2   | 2.02                     | 0.58              |
| 1:D:377:ILE:O    | 1:D:380:ALA:HB3  | 2.03                     | 0.58              |
| 1:U:283:LEU:HD11 | 1:U:322:GLU:HB3  | 1.85                     | 0.58              |
| 1:C:264:LYS:O    | 1:C:265:LYS:HB3  | 2.03                     | 0.58              |
| 2:I:82:TRP:CE2   | 2:I:88:LEU:HD13  | 2.38                     | 0.58              |
| 1:A:275:ARG:C    | 1:A:277:GLY:N    | 2.56                     | 0.58              |
| 1:U:235:ILE:HG22 | 1:U:236:ASN:N    | 2.18                     | 0.58              |
| 1:D:280:ARG:HG3  | 1:D:280:ARG:HH11 | 1.68                     | 0.58              |
| 1:V:286:VAL:HA   | 1:V:305:PHE:CE1  | 2.37                     | 0.58              |
| 2:Q:17:ASP:HB2   | 2:Q:164:ASN:HD22 | 1.68                     | 0.58              |
| 1:T:327:LEU:N    | 1:T:328:PRO:CD   | 2.64                     | 0.58              |
| 2:H:55:THR:HG21  | 2:H:89:ARG:NH2   | 2.18                     | 0.58              |
| 2:K:134:ALA:O    | 2:K:138:VAL:HG23 | 2.04                     | 0.58              |
| 1:F:4:MET:CE     | 1:F:9:ILE:HA     | 2.34                     | 0.58              |
| 2:L:8:ARG:O      | 2:L:9:ASN:HB2    | 2.03                     | 0.58              |
| 1:B:41:GLN:NE2   | 1:B:41:GLN:HA    | 2.18                     | 0.58              |
| 1:U:386:GLU:O    | 1:U:386:GLU:HG2  | 2.03                     | 0.58              |
| 1:B:17:ILE:N     | 1:B:17:ILE:HD12  | 2.18                     | 0.58              |
| 1:W:300:THR:HG22 | 1:W:303:ILE:HD11 | 1.84                     | 0.58              |
| 1:B:360:MET:CE   | 1:B:360:MET:HA   | 2.32                     | 0.58              |
| 1:B:283:LEU:CB   | 1:B:284:PRO:HD3  | 2.32                     | 0.58              |
| 1:W:51:LYS:HE2   | 1:X:356:TYR:OH   | 2.03                     | 0.58              |
| 1:U:23:ALA:HA    | 1:U:331:VAL:CG2  | 2.32                     | 0.58              |
| 1:C:264:LYS:HE3  | 1:C:264:LYS:H    | 1.68                     | 0.58              |
| 2:L:13:VAL:HG22  | 2:L:171:GLU:CB   | 2.33                     | 0.58              |
| 1:U:113:GLN:HG3  | 1:U:113:GLN:O    | 2.04                     | 0.58              |
| 1:A:322:GLU:OE2  | 1:A:322:GLU:N    | 2.35                     | 0.58              |
| 1:V:313:VAL:CG2  | 1:V:314:ALA:H    | 2.02                     | 0.58              |
| 1:W:23:ALA:HA    | 1:W:331:VAL:CG2  | 2.34                     | 0.58              |
| 1:B:264:LYS:NZ   | 1:B:279:GLN:NE2  | 2.44                     | 0.58              |
| 1:W:283:LEU:HD11 | 1:W:322:GLU:HB3  | 1.85                     | 0.58              |
| 1:U:37:ARG:HG2   | 1:U:37:ARG:HH11  | 1.69                     | 0.58              |
| 2:Q:164:ASN:N    | 2:Q:164:ASN:HD22 | 1.96                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:373:ALA:HB2  | 1:S:422:ASP:HA   | 1.85                     | 0.58              |
| 2:O:17:ASP:HB2   | 2:O:164:ASN:HD22 | 1.67                     | 0.58              |
| 2:O:72:LEU:O     | 2:O:76:VAL:HG23  | 2.02                     | 0.58              |
| 1:D:5:THR:H      | 1:D:8:GLU:HB3    | 1.69                     | 0.58              |
| 1:C:235:ILE:O    | 1:C:236:ASN:HB3  | 2.02                     | 0.58              |
| 2:N:72:LEU:O     | 2:N:76:VAL:HG23  | 2.03                     | 0.58              |
| 1:C:407:ILE:HD11 | 1:C:419:VAL:HG11 | 1.85                     | 0.58              |
| 1:V:386:GLU:O    | 1:V:386:GLU:HG2  | 2.03                     | 0.58              |
| 1:U:320:ILE:HD11 | 1:U:323:LEU:HD13 | 1.85                     | 0.58              |
| 1:W:63:LYS:HB2   | 3:W:460:ATP:O2B  | 2.03                     | 0.58              |
| 1:C:264:LYS:CE   | 1:C:279:GLN:HE22 | 2.16                     | 0.58              |
| 1:A:403:LEU:CD2  | 1:A:404:MET:SD   | 2.92                     | 0.58              |
| 1:E:405:ASP:HB3  | 1:E:406:LYS:HD2  | 1.85                     | 0.58              |
| 2:L:137:LEU:HD11 | 2:R:136:ALA:HB1  | 1.85                     | 0.58              |
| 1:U:327:LEU:N    | 1:U:328:PRO:CD   | 2.64                     | 0.58              |
| 1:S:355:GLN:OE1  | 1:X:48:VAL:HA    | 2.04                     | 0.58              |
| 1:X:23:ALA:HA    | 1:X:331:VAL:CG2  | 2.34                     | 0.58              |
| 1:T:37:ARG:HH11  | 1:T:37:ARG:HG2   | 1.69                     | 0.58              |
| 1:D:443:ILE:HG12 | 2:J:112:VAL:CG2  | 2.32                     | 0.58              |
| 1:B:250:GLN:HA   | 1:B:250:GLN:NE2  | 2.18                     | 0.58              |
| 1:T:120:ARG:O    | 1:T:124:GLU:HB3  | 2.04                     | 0.58              |
| 1:T:286:VAL:HA   | 1:T:305:PHE:CE1  | 2.38                     | 0.58              |
| 1:V:345:LEU:HD23 | 1:V:374:VAL:HG13 | 1.85                     | 0.58              |
| 1:S:386:GLU:HG2  | 1:S:386:GLU:O    | 2.04                     | 0.58              |
| 1:B:406:LYS:H    | 1:B:406:LYS:CD   | 2.09                     | 0.58              |
| 1:T:20:GLN:O     | 1:T:21:ALA:HB2   | 2.03                     | 0.58              |
| 2:J:1:THR:HG22   | 2:J:2:THR:N      | 2.19                     | 0.58              |
| 1:W:327:LEU:N    | 1:W:328:PRO:CD   | 2.64                     | 0.58              |
| 2:K:86:ARG:HG2   | 2:K:87:ALA:H     | 1.67                     | 0.58              |
| 1:W:259:ILE:O    | 1:W:262:ILE:HG12 | 2.04                     | 0.58              |
| 1:U:313:VAL:CG2  | 1:U:314:ALA:H    | 2.02                     | 0.58              |
| 1:W:27:VAL:HG21  | 1:W:66:ILE:CG2   | 2.33                     | 0.58              |
| 1:C:443:ILE:HG21 | 2:I:114:GLN:HG3  | 1.85                     | 0.58              |
| 1:U:5:THR:OG1    | 1:U:6:PRO:HD2    | 2.04                     | 0.58              |
| 2:K:37:LEU:HB2   | 2:K:42:VAL:CG2   | 2.33                     | 0.58              |
| 1:V:18:ILE:HG22  | 1:V:344:ILE:HG12 | 1.86                     | 0.58              |
| 1:W:442:PHE:CD1  | 1:W:442:PHE:N    | 2.72                     | 0.58              |
| 2:J:55:THR:O     | 2:J:59:LEU:HD13  | 2.04                     | 0.58              |
| 2:R:56:LEU:HD23  | 2:R:95:LEU:HD22  | 1.86                     | 0.58              |
| 1:E:403:LEU:HD22 | 1:E:404:MET:HG2  | 1.85                     | 0.58              |
| 1:T:80:LYS:HG3   | 1:T:255:PHE:HD2  | 1.66                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:55:THR:O     | 2:G:59:LEU:HD13  | 2.04                     | 0.58              |
| 1:C:403:LEU:CD2  | 1:C:404:MET:SD   | 2.92                     | 0.58              |
| 1:X:61:VAL:HA    | 1:X:336:LEU:HD21 | 1.85                     | 0.58              |
| 1:F:435:GLU:O    | 1:F:436:ASN:HB3  | 2.03                     | 0.58              |
| 1:A:34:ARG:CZ    | 1:A:251:ASN:HA   | 2.34                     | 0.58              |
| 1:E:313:VAL:HG23 | 1:E:314:ALA:H    | 1.69                     | 0.58              |
| 1:X:386:GLU:O    | 1:X:386:GLU:HG2  | 2.04                     | 0.58              |
| 1:F:406:LYS:H    | 1:F:406:LYS:CD   | 2.06                     | 0.57              |
| 2:R:7:ARG:HH21   | 2:R:103:SER:HB3  | 1.69                     | 0.57              |
| 2:N:17:ASP:HB2   | 2:N:164:ASN:HD22 | 1.68                     | 0.57              |
| 2:P:17:ASP:HB2   | 2:P:164:ASN:HD21 | 1.67                     | 0.57              |
| 1:X:27:VAL:HG21  | 1:X:66:ILE:HG21  | 1.86                     | 0.57              |
| 1:V:373:ALA:HB2  | 1:V:422:ASP:HA   | 1.86                     | 0.57              |
| 2:P:72:LEU:O     | 2:P:76:VAL:HG23  | 2.04                     | 0.57              |
| 2:K:8:ARG:O      | 2:K:9:ASN:HB2    | 2.04                     | 0.57              |
| 1:U:111:VAL:HG12 | 1:U:240:LEU:HD11 | 1.85                     | 0.57              |
| 2:K:82:TRP:CD1   | 2:K:88:LEU:HB3   | 2.39                     | 0.57              |
| 1:E:34:ARG:CZ    | 1:E:251:ASN:HA   | 2.34                     | 0.57              |
| 1:S:259:ILE:O    | 1:S:262:ILE:HG12 | 2.04                     | 0.57              |
| 1:W:80:LYS:HG3   | 1:W:255:PHE:HD2  | 1.68                     | 0.57              |
| 2:R:72:LEU:O     | 2:R:76:VAL:HG23  | 2.03                     | 0.57              |
| 1:T:27:VAL:HG21  | 1:T:66:ILE:HG21  | 1.85                     | 0.57              |
| 1:S:80:LYS:HG3   | 1:S:255:PHE:HD2  | 1.69                     | 0.57              |
| 2:G:144:SER:HB3  | 2:G:147:GLU:CG   | 2.32                     | 0.57              |
| 1:W:37:ARG:NH1   | 1:W:37:ARG:HG2   | 2.18                     | 0.57              |
| 1:V:23:ALA:HA    | 1:V:331:VAL:CG2  | 2.34                     | 0.57              |
| 1:V:333:LEU:HD23 | 1:V:333:LEU:N    | 2.18                     | 0.57              |
| 1:T:227:ILE:HG23 | 1:T:228:ASP:N    | 2.18                     | 0.57              |
| 1:B:407:ILE:O    | 1:B:411:ALA:HB2  | 2.04                     | 0.57              |
| 1:T:240:LEU:HD12 | 1:T:243:LYS:HB3  | 1.86                     | 0.57              |
| 1:E:54:LEU:HG    | 1:E:56:ILE:HD11  | 1.86                     | 0.57              |
| 1:X:259:ILE:O    | 1:X:262:ILE:HG12 | 2.03                     | 0.57              |
| 2:M:120:ILE:O    | 2:M:121:LEU:HD23 | 2.03                     | 0.57              |
| 2:I:17:ASP:O     | 2:I:33:LYS:HD2   | 2.03                     | 0.57              |
| 1:X:63:LYS:HZ2   | 1:X:308:SER:HB2  | 1.68                     | 0.57              |
| 1:A:275:ARG:O    | 1:A:277:GLY:N    | 2.37                     | 0.57              |
| 1:A:112:ARG:C    | 1:A:114:GLN:H    | 2.07                     | 0.57              |
| 1:S:79:ILE:HG22  | 1:S:103:LEU:HD13 | 1.86                     | 0.57              |
| 1:U:23:ALA:O     | 1:U:27:VAL:HG23  | 2.04                     | 0.57              |
| 1:S:333:LEU:HD23 | 1:S:333:LEU:N    | 2.19                     | 0.57              |
| 2:H:137:LEU:HD11 | 2:N:136:ALA:HB1  | 1.85                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:K:52:ASP:CA   | 2:K:55:THR:HG23  | 2.34                     | 0.57              |
| 1:X:327:LEU:N   | 1:X:328:PRO:CD   | 2.67                     | 0.57              |
| 1:F:60:GLY:HA2  | 3:F:455:ATP:O1B  | 2.04                     | 0.57              |
| 1:X:20:GLN:OE1  | 1:X:333:LEU:HB3  | 2.04                     | 0.57              |
| 2:O:37:LEU:HB2  | 2:O:42:VAL:HG23  | 1.86                     | 0.57              |
| 1:V:27:VAL:HG21 | 1:V:66:ILE:CG2   | 2.34                     | 0.57              |
| 1:A:41:GLN:HE21 | 1:A:41:GLN:CA    | 2.16                     | 0.57              |
| 1:C:54:LEU:HG   | 1:C:56:ILE:CD1   | 2.35                     | 0.57              |
| 1:A:315:ARG:O   | 1:A:318:ASP:HB2  | 2.04                     | 0.57              |
| 1:A:316:PRO:C   | 1:A:318:ASP:H    | 2.08                     | 0.57              |
| 2:P:49:GLY:O    | 2:P:50:THR:C     | 2.43                     | 0.57              |
| 2:M:17:ASP:HB2  | 2:M:164:ASN:HD21 | 1.66                     | 0.57              |
| 1:A:435:GLU:HG3 | 1:A:436:ASN:N    | 2.16                     | 0.57              |
| 1:T:328:PRO:HB3 | 1:U:398:THR:HA   | 1.85                     | 0.57              |
| 1:U:328:PRO:HB3 | 1:V:398:THR:HA   | 1.85                     | 0.57              |
| 1:V:370:THR:CG2 | 1:V:422:ASP:HA   | 2.35                     | 0.57              |
| 1:E:58:PRO:O    | 1:E:63:LYS:NZ    | 2.28                     | 0.57              |
| 1:C:104:THR:HA  | 1:C:248:VAL:CG2  | 2.32                     | 0.57              |
| 1:C:366:ASN:O   | 1:C:418:THR:HA   | 2.03                     | 0.57              |
| 2:I:86:ARG:O    | 2:I:87:ALA:HB2   | 2.04                     | 0.57              |
| 1:A:27:VAL:HB   | 1:A:70:LEU:HD22  | 1.86                     | 0.57              |
| 1:E:52:ASN:O    | 1:E:328:PRO:HD2  | 2.05                     | 0.57              |
| 2:J:17:ASP:HB2  | 2:J:164:ASN:HD22 | 1.69                     | 0.57              |
| 2:K:1:THR:HG23  | 2:K:33:LYS:NZ    | 2.19                     | 0.57              |
| 1:E:41:GLN:HA   | 1:E:41:GLN:HE21  | 1.68                     | 0.57              |
| 1:C:54:LEU:HD12 | 1:C:307:ALA:O    | 2.04                     | 0.57              |
| 1:V:341:PHE:O   | 1:V:345:LEU:HB2  | 2.05                     | 0.57              |
| 1:B:235:ILE:O   | 1:B:236:ASN:HB3  | 2.05                     | 0.57              |
| 1:X:79:ILE:HG22 | 1:X:103:LEU:HD13 | 1.86                     | 0.57              |
| 1:E:264:LYS:O   | 1:E:265:LYS:HB3  | 2.05                     | 0.57              |
| 1:V:327:LEU:N   | 1:V:328:PRO:CD   | 2.67                     | 0.57              |
| 2:K:17:ASP:HB2  | 2:K:164:ASN:HD22 | 1.67                     | 0.57              |
| 1:E:280:ARG:HG3 | 1:E:280:ARG:NH1  | 2.16                     | 0.57              |
| 1:D:333:LEU:N   | 1:D:333:LEU:HD12 | 2.19                     | 0.57              |
| 2:N:37:LEU:HB2  | 2:N:42:VAL:HG23  | 1.87                     | 0.57              |
| 2:M:1:THR:HG23  | 2:M:33:LYS:HD3   | 1.86                     | 0.57              |
| 2:I:115:PRO:HB2 | 2:I:119:GLN:HA   | 1.87                     | 0.57              |
| 1:B:293:THR:C   | 1:B:295:HIS:H    | 2.08                     | 0.57              |
| 1:D:6:PRO:HD3   | 1:D:32:ARG:HG2   | 1.87                     | 0.57              |
| 1:E:409:PHE:CZ  | 1:F:25:ARG:HG3   | 2.40                     | 0.57              |
| 1:E:41:GLN:HE21 | 1:E:41:GLN:CA    | 2.18                     | 0.57              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:86:ARG:O     | 2:L:87:ALA:CB    | 2.53                     | 0.57              |
| 2:R:37:LEU:HB2   | 2:R:42:VAL:HG23  | 1.87                     | 0.57              |
| 1:D:406:LYS:N    | 1:D:406:LYS:HD2  | 2.10                     | 0.57              |
| 1:T:20:GLN:OE1   | 1:T:333:LEU:HB3  | 2.05                     | 0.57              |
| 2:M:3:ILE:O      | 2:M:122:ALA:HA   | 2.04                     | 0.57              |
| 1:D:382:PHE:C    | 1:D:382:PHE:CD2  | 2.78                     | 0.57              |
| 2:M:56:LEU:HD23  | 2:M:95:LEU:HD22  | 1.86                     | 0.57              |
| 2:Q:120:ILE:O    | 2:Q:121:LEU:HD23 | 2.05                     | 0.57              |
| 2:R:17:ASP:HB2   | 2:R:164:ASN:HD22 | 1.70                     | 0.57              |
| 1:E:38:MET:HG3   | 1:E:45:ARG:NH1   | 2.20                     | 0.57              |
| 1:E:360:MET:HE2  | 1:E:360:MET:N    | 2.20                     | 0.56              |
| 1:S:327:LEU:N    | 1:S:328:PRO:CD   | 2.64                     | 0.56              |
| 1:X:37:ARG:HG2   | 1:X:37:ARG:HH11  | 1.69                     | 0.56              |
| 1:V:303:ILE:HG22 | 1:V:304:LEU:N    | 2.20                     | 0.56              |
| 1:A:370:THR:HG23 | 1:A:421:ILE:O    | 2.04                     | 0.56              |
| 1:B:245:ILE:HG23 | 1:B:298:VAL:HG12 | 1.87                     | 0.56              |
| 2:G:38:TYR:CD1   | 2:G:69:GLY:HA3   | 2.39                     | 0.56              |
| 1:V:17:ILE:HD13  | 1:V:66:ILE:CG1   | 2.35                     | 0.56              |
| 1:C:237:PRO:CB   | 1:C:241:LYS:HZ1  | 2.18                     | 0.56              |
| 1:A:25:ARG:O     | 1:A:28:ALA:N     | 2.38                     | 0.56              |
| 1:S:283:LEU:HD11 | 1:S:322:GLU:HB3  | 1.88                     | 0.56              |
| 1:F:341:PHE:O    | 1:F:345:LEU:HB2  | 2.04                     | 0.56              |
| 1:W:324:GLN:HE22 | 1:X:389:GLU:HG2  | 1.70                     | 0.56              |
| 2:O:56:LEU:HD21  | 2:O:95:LEU:HB2   | 1.87                     | 0.56              |
| 2:P:37:LEU:HB2   | 2:P:42:VAL:HG23  | 1.87                     | 0.56              |
| 1:V:59:THR:HG23  | 3:V:459:ATP:O1G  | 2.06                     | 0.56              |
| 1:U:79:ILE:HG22  | 1:U:103:LEU:HD13 | 1.86                     | 0.56              |
| 1:V:79:ILE:HG22  | 1:V:103:LEU:HD13 | 1.86                     | 0.56              |
| 2:J:8:ARG:O      | 2:J:9:ASN:HB2    | 2.05                     | 0.56              |
| 2:O:120:ILE:O    | 2:O:121:LEU:HD23 | 2.05                     | 0.56              |
| 2:L:36:ARG:NH1   | 2:L:170:GLU:OE2  | 2.39                     | 0.56              |
| 2:K:71:LEU:C     | 2:K:71:LEU:HD13  | 2.26                     | 0.56              |
| 1:D:256:ILE:HG21 | 1:D:259:ILE:HD12 | 1.85                     | 0.56              |
| 2:H:8:ARG:O      | 2:H:9:ASN:HB2    | 2.05                     | 0.56              |
| 1:U:315:ARG:HB3  | 1:U:316:PRO:HD2  | 1.87                     | 0.56              |
| 1:F:373:ALA:O    | 1:F:377:ILE:HG13 | 2.06                     | 0.56              |
| 1:X:283:LEU:HB3  | 1:X:284:PRO:HD3  | 1.88                     | 0.56              |
| 1:A:435:GLU:C    | 1:A:437:GLU:H    | 2.08                     | 0.56              |
| 2:K:49:GLY:O     | 2:K:50:THR:C     | 2.42                     | 0.56              |
| 2:H:17:ASP:HB2   | 2:H:164:ASN:HD22 | 1.68                     | 0.56              |
| 2:H:105:ILE:HG22 | 2:H:113:VAL:O    | 2.05                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:303:ILE:HG22 | 1:S:304:LEU:N    | 2.21                     | 0.56              |
| 1:S:300:THR:HG22 | 1:S:303:ILE:HD11 | 1.86                     | 0.56              |
| 1:A:104:THR:HA   | 1:A:248:VAL:CG2  | 2.35                     | 0.56              |
| 1:B:37:ARG:HH22  | 1:B:250:GLN:HE22 | 1.52                     | 0.56              |
| 2:G:71:LEU:HD13  | 2:G:71:LEU:C     | 2.26                     | 0.56              |
| 1:V:39:GLN:HB2   | 1:W:362:THR:HG21 | 1.86                     | 0.56              |
| 2:M:89:ARG:HH11  | 2:N:87:ALA:HB2   | 1.70                     | 0.56              |
| 1:E:370:THR:O    | 1:E:373:ALA:HB3  | 2.06                     | 0.56              |
| 1:W:112:ARG:O    | 1:W:116:ILE:HB   | 2.06                     | 0.56              |
| 1:S:68:ARG:HG3   | 1:S:68:ARG:HH11  | 1.70                     | 0.56              |
| 1:T:283:LEU:HD11 | 1:T:322:GLU:HB3  | 1.88                     | 0.56              |
| 1:D:403:LEU:CD2  | 1:D:404:MET:SD   | 2.93                     | 0.56              |
| 1:C:65:GLU:HG3   | 3:C:452:ATP:H2'  | 1.88                     | 0.56              |
| 1:E:352:LEU:HD13 | 1:E:400:MET:HG3  | 1.87                     | 0.56              |
| 1:W:369:PHE:CE2  | 1:W:421:ILE:HD12 | 2.33                     | 0.56              |
| 1:S:20:GLN:OE1   | 1:S:333:LEU:HB3  | 2.05                     | 0.56              |
| 1:S:18:ILE:HG22  | 1:S:344:ILE:HG12 | 1.86                     | 0.56              |
| 2:R:8:ARG:O      | 2:R:9:ASN:HB2    | 2.04                     | 0.56              |
| 2:O:8:ARG:O      | 2:O:9:ASN:HB2    | 2.05                     | 0.56              |
| 2:G:83:ARG:HB3   | 2:H:55:THR:HB    | 1.88                     | 0.56              |
| 1:X:227:ILE:HG23 | 1:X:228:ASP:N    | 2.20                     | 0.56              |
| 1:V:65:GLU:HG2   | 3:V:459:ATP:H5'2 | 1.88                     | 0.56              |
| 2:J:86:ARG:O     | 2:J:87:ALA:CB    | 2.53                     | 0.56              |
| 1:E:264:LYS:NZ   | 1:E:319:LEU:HA   | 2.21                     | 0.56              |
| 2:I:7:ARG:NE     | 2:I:119:GLN:OE1  | 2.38                     | 0.56              |
| 1:C:52:ASN:HD21  | 1:C:305:PHE:H    | 1.49                     | 0.56              |
| 1:B:341:PHE:HA   | 1:B:344:ILE:HG12 | 1.87                     | 0.56              |
| 2:N:56:LEU:HD21  | 2:N:95:LEU:HB2   | 1.88                     | 0.56              |
| 1:A:366:ASN:O    | 1:A:418:THR:HA   | 2.05                     | 0.56              |
| 2:O:17:ASP:HB2   | 2:O:164:ASN:HD21 | 1.68                     | 0.56              |
| 1:S:23:ALA:HA    | 1:S:331:VAL:CG2  | 2.35                     | 0.56              |
| 1:V:328:PRO:HB3  | 1:W:398:THR:HA   | 1.86                     | 0.56              |
| 2:J:46:PHE:HB3   | 2:J:95:LEU:CD2   | 2.35                     | 0.56              |
| 1:U:247:ALA:O    | 1:U:251:ASN:HB2  | 2.06                     | 0.56              |
| 1:S:108:MET:HE2  | 1:S:244:ALA:HB1  | 1.87                     | 0.56              |
| 1:T:300:THR:HG22 | 1:T:303:ILE:HD11 | 1.88                     | 0.56              |
| 1:V:37:ARG:HG2   | 1:V:37:ARG:NH1   | 2.19                     | 0.56              |
| 1:D:315:ARG:O    | 1:D:318:ASP:HB2  | 2.05                     | 0.56              |
| 2:N:7:ARG:HE     | 2:N:119:GLN:NE2  | 2.04                     | 0.56              |
| 1:F:369:PHE:CE2  | 1:F:421:ILE:HD12 | 2.40                     | 0.56              |
| 2:P:56:LEU:CD2   | 2:P:95:LEU:HD22  | 2.35                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:233:LYS:C    | 1:S:235:ILE:H    | 2.08                     | 0.56              |
| 1:X:373:ALA:HB2  | 1:X:422:ASP:HA   | 1.87                     | 0.56              |
| 2:K:17:ASP:OD2   | 2:K:33:LYS:HE3   | 2.05                     | 0.56              |
| 1:D:373:ALA:O    | 1:D:377:ILE:HG13 | 2.05                     | 0.56              |
| 1:S:349:HIS:O    | 1:S:350:ALA:HB3  | 2.06                     | 0.56              |
| 2:M:83:ARG:HG2   | 2:R:55:THR:HG22  | 1.87                     | 0.56              |
| 1:C:20:GLN:HE21  | 1:C:20:GLN:H     | 1.54                     | 0.56              |
| 1:B:236:ASN:O    | 1:B:238:GLU:N    | 2.38                     | 0.56              |
| 2:O:3:ILE:O      | 2:O:122:ALA:HA   | 2.05                     | 0.56              |
| 1:A:264:LYS:HZ1  | 1:A:279:GLN:NE2  | 2.00                     | 0.56              |
| 1:U:17:ILE:HD13  | 1:U:66:ILE:HG12  | 1.87                     | 0.56              |
| 2:M:95:LEU:O     | 2:M:105:ILE:HA   | 2.06                     | 0.56              |
| 1:E:52:ASN:HD22  | 1:E:305:PHE:N    | 2.01                     | 0.56              |
| 1:T:27:VAL:HG21  | 1:T:66:ILE:CG2   | 2.36                     | 0.56              |
| 2:M:164:ASN:N    | 2:M:164:ASN:HD22 | 1.95                     | 0.56              |
| 1:T:353:THR:HG22 | 1:T:369:PHE:CD1  | 2.40                     | 0.56              |
| 1:U:54:LEU:HD21  | 1:U:327:LEU:HD22 | 1.87                     | 0.56              |
| 1:U:373:ALA:HB2  | 1:U:422:ASP:HA   | 1.88                     | 0.56              |
| 2:R:5:SER:CB     | 2:R:14:VAL:HG22  | 2.35                     | 0.56              |
| 1:V:17:ILE:HD13  | 1:V:66:ILE:HG12  | 1.88                     | 0.56              |
| 1:T:430:LEU:HG   | 1:T:431:GLY:H    | 1.70                     | 0.56              |
| 1:F:283:LEU:HB2  | 1:F:284:PRO:HD3  | 1.88                     | 0.56              |
| 1:C:41:GLN:NE2   | 1:C:41:GLN:HA    | 2.21                     | 0.56              |
| 2:M:115:PRO:HB3  | 2:M:119:GLN:CA   | 2.34                     | 0.56              |
| 1:C:443:ILE:HG12 | 2:I:112:VAL:CG2  | 2.35                     | 0.56              |
| 2:K:144:SER:HB3  | 2:K:147:GLU:CG   | 2.35                     | 0.56              |
| 1:V:48:VAL:HG21  | 1:W:359:LEU:HD11 | 1.88                     | 0.56              |
| 1:F:438:ASP:O    | 1:F:439:LEU:C    | 2.43                     | 0.56              |
| 1:C:250:GLN:NE2  | 1:C:250:GLN:HA   | 2.20                     | 0.56              |
| 1:V:111:VAL:O    | 1:V:115:GLU:HB2  | 2.05                     | 0.56              |
| 1:F:41:GLN:NE2   | 1:F:41:GLN:HA    | 2.21                     | 0.56              |
| 1:V:283:LEU:HB3  | 1:V:284:PRO:HD3  | 1.87                     | 0.56              |
| 1:F:370:THR:HG23 | 1:F:421:ILE:O    | 2.06                     | 0.56              |
| 2:R:56:LEU:CD2   | 2:R:95:LEU:HD13  | 2.36                     | 0.56              |
| 1:E:360:MET:CE   | 1:E:360:MET:HA   | 2.36                     | 0.56              |
| 1:T:63:LYS:HZ2   | 1:T:308:SER:HB2  | 1.69                     | 0.56              |
| 2:N:17:ASP:HB2   | 2:N:164:ASN:HD21 | 1.66                     | 0.56              |
| 1:X:54:LEU:HD21  | 1:X:327:LEU:HD22 | 1.86                     | 0.56              |
| 1:E:58:PRO:HD2   | 1:E:61:VAL:HG21  | 1.88                     | 0.56              |
| 1:D:370:THR:O    | 1:D:373:ALA:HB3  | 2.06                     | 0.56              |
| 1:D:437:GLU:O    | 1:D:438:ASP:C    | 2.44                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:111:VAL:HG21 | 1:D:244:ALA:HA   | 1.88                     | 0.56              |
| 1:F:240:LEU:O    | 1:F:243:LYS:N    | 2.31                     | 0.56              |
| 1:T:435:GLU:O    | 1:T:436:ASN:O    | 2.22                     | 0.56              |
| 1:S:439:LEU:N    | 1:S:439:LEU:HD23 | 2.19                     | 0.56              |
| 2:Q:56:LEU:CD2   | 2:Q:95:LEU:HD22  | 2.36                     | 0.56              |
| 2:Q:8:ARG:O      | 2:Q:9:ASN:HB2    | 2.05                     | 0.56              |
| 2:R:128:ASN:HA   | 2:R:131:LEU:HB3  | 1.88                     | 0.56              |
| 2:J:115:PRO:HB2  | 2:J:119:GLN:HA   | 1.88                     | 0.56              |
| 1:S:37:ARG:NH1   | 1:S:37:ARG:HG2   | 2.20                     | 0.56              |
| 1:B:37:ARG:HA    | 1:B:40:LEU:HD12  | 1.88                     | 0.56              |
| 1:A:20:GLN:OE1   | 1:A:333:LEU:HB3  | 2.06                     | 0.56              |
| 2:L:86:ARG:O     | 2:L:87:ALA:HB2   | 2.05                     | 0.56              |
| 2:J:43:LEU:O     | 2:J:97:VAL:HA    | 2.05                     | 0.56              |
| 1:B:349:HIS:O    | 1:B:350:ALA:HB3  | 2.06                     | 0.56              |
| 2:H:38:TYR:CE1   | 2:H:69:GLY:HA3   | 2.41                     | 0.56              |
| 1:D:41:GLN:NE2   | 1:D:41:GLN:HA    | 2.21                     | 0.56              |
| 1:V:283:LEU:HD13 | 1:V:323:LEU:HD12 | 1.88                     | 0.55              |
| 2:Q:56:LEU:HD21  | 2:Q:95:LEU:HB2   | 1.88                     | 0.55              |
| 1:S:370:THR:CG2  | 1:S:422:ASP:HA   | 2.36                     | 0.55              |
| 1:S:17:ILE:HG23  | 3:S:456:ATP:N6   | 2.21                     | 0.55              |
| 1:C:341:PHE:HA   | 1:C:344:ILE:HG12 | 1.89                     | 0.55              |
| 2:Q:37:LEU:HB2   | 2:Q:42:VAL:HG23  | 1.88                     | 0.55              |
| 1:B:391:ILE:HG22 | 1:C:321:PRO:HB3  | 1.88                     | 0.55              |
| 1:E:437:GLU:O    | 1:E:438:ASP:O    | 2.23                     | 0.55              |
| 1:A:414:MET:O    | 1:A:414:MET:HG2  | 2.06                     | 0.55              |
| 1:U:27:VAL:HG21  | 1:U:66:ILE:CG2   | 2.36                     | 0.55              |
| 1:B:352:LEU:HD13 | 1:B:400:MET:CG   | 2.35                     | 0.55              |
| 1:S:5:THR:OG1    | 1:S:6:PRO:HD2    | 2.06                     | 0.55              |
| 1:U:120:ARG:HG3  | 1:U:232:ALA:CB   | 2.36                     | 0.55              |
| 2:G:5:SER:HB2    | 2:G:14:VAL:HG22  | 1.87                     | 0.55              |
| 1:A:118:LYS:C    | 1:A:120:ARG:H    | 2.10                     | 0.55              |
| 1:B:113:GLN:HG2  | 1:B:113:GLN:O    | 2.05                     | 0.55              |
| 1:T:283:LEU:HB3  | 1:T:284:PRO:HD3  | 1.88                     | 0.55              |
| 1:T:373:ALA:HB2  | 1:T:422:ASP:HA   | 1.88                     | 0.55              |
| 1:F:250:GLN:HE21 | 1:F:250:GLN:CA   | 2.19                     | 0.55              |
| 1:C:338:ALA:N    | 1:C:382:PHE:HD1  | 2.03                     | 0.55              |
| 1:A:37:ARG:CG    | 1:A:38:MET:N     | 2.69                     | 0.55              |
| 1:D:316:PRO:C    | 1:D:318:ASP:H    | 2.09                     | 0.55              |
| 1:F:31:LEU:HD21  | 1:F:74:ALA:HB2   | 1.88                     | 0.55              |
| 2:H:115:PRO:HG3  | 2:H:121:LEU:HD11 | 1.88                     | 0.55              |
| 2:P:56:LEU:HD21  | 2:P:95:LEU:HB2   | 1.89                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:55:THR:O     | 2:I:59:LEU:HD13  | 2.06                     | 0.55              |
| 1:S:55:MET:HA    | 1:S:331:VAL:HG13 | 1.88                     | 0.55              |
| 1:B:360:MET:HE3  | 1:C:36:ARG:NH1   | 2.22                     | 0.55              |
| 2:J:105:ILE:HG22 | 2:J:113:VAL:O    | 2.07                     | 0.55              |
| 1:T:341:PHE:O    | 1:T:345:LEU:HB2  | 2.07                     | 0.55              |
| 1:W:341:PHE:O    | 1:W:345:LEU:HB2  | 2.07                     | 0.55              |
| 1:W:68:ARG:HG3   | 1:W:68:ARG:HH11  | 1.71                     | 0.55              |
| 1:A:53:ILE:HG22  | 1:A:54:LEU:N     | 2.21                     | 0.55              |
| 2:K:43:LEU:O     | 2:K:97:VAL:HA    | 2.07                     | 0.55              |
| 1:F:17:ILE:HG12  | 1:F:66:ILE:HG13  | 1.89                     | 0.55              |
| 1:W:303:ILE:HG22 | 1:W:304:LEU:N    | 2.20                     | 0.55              |
| 1:D:358:ALA:O    | 1:D:361:ALA:HB3  | 2.07                     | 0.55              |
| 1:X:60:GLY:HA3   | 1:X:392:GLY:HA3  | 1.88                     | 0.55              |
| 2:M:87:ALA:HB2   | 2:R:89:ARG:HH11  | 1.72                     | 0.55              |
| 1:U:280:ARG:HH22 | 1:V:261:LYS:HE3  | 1.72                     | 0.55              |
| 1:C:322:GLU:OE2  | 1:C:322:GLU:N    | 2.39                     | 0.55              |
| 1:W:442:PHE:H    | 1:W:442:PHE:HD1  | 1.53                     | 0.55              |
| 1:T:313:VAL:CG2  | 1:T:314:ALA:H    | 2.00                     | 0.55              |
| 1:F:367:ILE:HD11 | 1:F:421:ILE:CD1  | 2.35                     | 0.55              |
| 1:A:404:MET:O    | 1:A:408:SER:HB2  | 2.07                     | 0.55              |
| 2:M:105:ILE:HG22 | 2:M:113:VAL:O    | 2.05                     | 0.55              |
| 1:F:65:GLU:HG3   | 3:F:455:ATP:H2'  | 1.88                     | 0.55              |
| 2:M:37:LEU:HB2   | 2:M:42:VAL:HG23  | 1.88                     | 0.55              |
| 2:O:128:ASN:HA   | 2:O:131:LEU:HB3  | 1.88                     | 0.55              |
| 1:D:421:ILE:HA   | 1:D:425:TYR:HD1  | 1.70                     | 0.55              |
| 1:F:360:MET:HA   | 1:F:360:MET:CE   | 2.36                     | 0.55              |
| 1:F:443:ILE:HG12 | 2:L:112:VAL:CG2  | 2.35                     | 0.55              |
| 1:C:4:MET:HE3    | 1:C:8:GLU:HG2    | 1.88                     | 0.55              |
| 1:F:275:ARG:O    | 1:F:277:GLY:N    | 2.40                     | 0.55              |
| 1:A:245:ILE:HG23 | 1:A:298:VAL:HG12 | 1.88                     | 0.55              |
| 1:C:275:ARG:C    | 1:C:277:GLY:N    | 2.59                     | 0.55              |
| 1:C:54:LEU:HG    | 1:C:56:ILE:HD11  | 1.89                     | 0.55              |
| 1:W:48:VAL:HG23  | 1:X:355:GLN:OE1  | 2.06                     | 0.55              |
| 1:T:349:HIS:O    | 1:T:350:ALA:HB3  | 2.07                     | 0.55              |
| 1:B:315:ARG:O    | 1:B:318:ASP:HB2  | 2.07                     | 0.55              |
| 1:E:357:LYS:HE3  | 1:E:367:ILE:O    | 2.06                     | 0.55              |
| 2:M:128:ASN:HA   | 2:M:131:LEU:HB3  | 1.89                     | 0.55              |
| 2:G:55:THR:HG22  | 2:L:83:ARG:HG2   | 1.89                     | 0.55              |
| 1:D:20:GLN:CA    | 1:D:20:GLN:NE2   | 2.69                     | 0.55              |
| 2:P:55:THR:HG22  | 2:Q:83:ARG:CG    | 2.36                     | 0.55              |
| 2:I:8:ARG:O      | 2:I:9:ASN:HB2    | 2.06                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:98:SER:HA    | 1:T:101:ARG:NH1  | 2.22                     | 0.55              |
| 1:V:362:THR:O    | 1:V:362:THR:HG22 | 2.07                     | 0.55              |
| 1:V:283:LEU:HD11 | 1:V:322:GLU:HB3  | 1.88                     | 0.55              |
| 2:R:56:LEU:HD21  | 2:R:95:LEU:HB2   | 1.87                     | 0.55              |
| 1:C:406:LYS:H    | 1:C:406:LYS:CD   | 2.13                     | 0.55              |
| 2:O:56:LEU:CD2   | 2:O:95:LEU:HD22  | 2.37                     | 0.55              |
| 1:S:353:THR:HG22 | 1:S:369:PHE:CD1  | 2.42                     | 0.55              |
| 2:L:17:ASP:O     | 2:L:33:LYS:HD2   | 2.06                     | 0.55              |
| 2:J:57:PHE:HA    | 2:J:95:LEU:HD11  | 1.88                     | 0.55              |
| 1:T:315:ARG:HB3  | 1:T:316:PRO:HD2  | 1.89                     | 0.55              |
| 1:D:250:GLN:HE21 | 1:D:250:GLN:CA   | 2.18                     | 0.55              |
| 1:E:104:THR:HA   | 1:E:248:VAL:CG2  | 2.36                     | 0.55              |
| 1:X:349:HIS:O    | 1:X:350:ALA:HB3  | 2.07                     | 0.55              |
| 1:T:259:ILE:O    | 1:T:262:ILE:HG12 | 2.05                     | 0.55              |
| 1:F:403:LEU:C    | 1:F:405:ASP:H    | 2.10                     | 0.55              |
| 1:B:316:PRO:C    | 1:B:318:ASP:H    | 2.08                     | 0.55              |
| 1:E:355:GLN:O    | 1:E:359:LEU:HD23 | 2.07                     | 0.55              |
| 1:A:439:LEU:HD23 | 1:A:443:ILE:HD12 | 1.89                     | 0.55              |
| 1:S:17:ILE:HD13  | 1:S:66:ILE:CG1   | 2.37                     | 0.55              |
| 2:R:1:THR:HG23   | 2:R:33:LYS:HD3   | 1.87                     | 0.55              |
| 1:F:104:THR:HA   | 1:F:248:VAL:CG2  | 2.36                     | 0.55              |
| 1:V:55:MET:HA    | 1:V:331:VAL:HG13 | 1.89                     | 0.55              |
| 1:T:61:VAL:HA    | 1:T:336:LEU:HD21 | 1.89                     | 0.55              |
| 1:D:41:GLN:HE21  | 1:D:41:GLN:HA    | 1.71                     | 0.55              |
| 1:U:98:SER:HA    | 1:U:101:ARG:NH1  | 2.22                     | 0.55              |
| 1:D:366:ASN:HB3  | 1:D:418:THR:HG22 | 1.88                     | 0.55              |
| 1:D:428:ASP:O    | 1:D:430:LEU:N    | 2.40                     | 0.55              |
| 1:V:68:ARG:HH11  | 1:V:68:ARG:HG3   | 1.72                     | 0.55              |
| 1:W:17:ILE:HD13  | 1:W:66:ILE:CG1   | 2.36                     | 0.55              |
| 2:O:56:LEU:CD2   | 2:O:95:LEU:HD13  | 2.37                     | 0.55              |
| 2:Q:128:ASN:HA   | 2:Q:131:LEU:HB3  | 1.89                     | 0.55              |
| 2:H:37:LEU:HB2   | 2:H:42:VAL:CG2   | 2.37                     | 0.55              |
| 1:W:373:ALA:HB2  | 1:W:422:ASP:HA   | 1.87                     | 0.55              |
| 1:S:393:ALA:HB3  | 3:S:456:ATP:C1'  | 2.35                     | 0.55              |
| 2:N:8:ARG:O      | 2:N:9:ASN:HB2    | 2.07                     | 0.55              |
| 2:P:4:VAL:HG12   | 2:P:153:LEU:HD21 | 1.89                     | 0.55              |
| 2:I:1:THR:HG23   | 2:I:33:LYS:NZ    | 2.22                     | 0.55              |
| 1:X:27:VAL:HG21  | 1:X:66:ILE:CG2   | 2.37                     | 0.55              |
| 1:T:280:ARG:HH22 | 1:U:261:LYS:HE3  | 1.71                     | 0.55              |
| 2:P:20:VAL:HG21  | 1:W:444:LEU:HD21 | 1.87                     | 0.55              |
| 2:N:105:ILE:HG22 | 2:N:113:VAL:O    | 2.06                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:37:ARG:HG2   | 1:U:37:ARG:NH1   | 2.22                     | 0.54              |
| 1:X:55:MET:HA    | 1:X:331:VAL:HG13 | 1.89                     | 0.54              |
| 2:G:78:LEU:O     | 2:G:81:ASP:HB2   | 2.06                     | 0.54              |
| 1:C:38:MET:HG3   | 1:C:45:ARG:NH1   | 2.21                     | 0.54              |
| 1:U:341:PHE:O    | 1:U:345:LEU:HB2  | 2.07                     | 0.54              |
| 2:N:55:THR:HG22  | 2:O:83:ARG:CB    | 2.37                     | 0.54              |
| 1:D:249:GLU:OE1  | 1:D:299:LYS:HG3  | 2.07                     | 0.54              |
| 1:C:76:ALA:HB1   | 1:C:251:ASN:O    | 2.07                     | 0.54              |
| 1:W:79:ILE:HG22  | 1:W:103:LEU:HD13 | 1.88                     | 0.54              |
| 1:D:264:LYS:HZ1  | 1:D:279:GLN:NE2  | 1.92                     | 0.54              |
| 1:S:18:ILE:CG2   | 1:S:344:ILE:HG13 | 2.36                     | 0.54              |
| 2:P:17:ASP:HB2   | 2:P:164:ASN:HD22 | 1.70                     | 0.54              |
| 2:L:38:TYR:CD1   | 2:L:69:GLY:HA3   | 2.42                     | 0.54              |
| 1:X:63:LYS:HZ2   | 1:X:63:LYS:HB2   | 1.71                     | 0.54              |
| 1:S:96:VAL:CG1   | 1:S:282:LEU:HD12 | 2.37                     | 0.54              |
| 1:B:360:MET:N    | 1:B:360:MET:HE2  | 2.21                     | 0.54              |
| 2:H:105:ILE:HG23 | 2:H:105:ILE:O    | 2.06                     | 0.54              |
| 1:S:362:THR:O    | 1:S:362:THR:HG22 | 2.06                     | 0.54              |
| 1:E:353:THR:O    | 1:E:354:GLU:C    | 2.42                     | 0.54              |
| 1:S:430:LEU:HG   | 1:S:431:GLY:H    | 1.72                     | 0.54              |
| 1:A:264:LYS:CE   | 1:A:279:GLN:HE22 | 2.17                     | 0.54              |
| 1:A:362:THR:HG21 | 1:B:39:GLN:HG2   | 1.90                     | 0.54              |
| 2:P:105:ILE:HG22 | 2:P:113:VAL:O    | 2.07                     | 0.54              |
| 1:T:55:MET:HA    | 1:T:331:VAL:HG13 | 1.89                     | 0.54              |
| 1:A:61:VAL:HA    | 1:A:336:LEU:HD22 | 1.90                     | 0.54              |
| 1:T:369:PHE:CE2  | 1:T:421:ILE:HD12 | 2.33                     | 0.54              |
| 2:H:1:THR:HG23   | 2:H:33:LYS:NZ    | 2.22                     | 0.54              |
| 1:C:439:LEU:O    | 1:C:440:SER:C    | 2.45                     | 0.54              |
| 1:T:303:ILE:HG22 | 1:T:304:LEU:N    | 2.18                     | 0.54              |
| 1:A:37:ARG:HH12  | 1:A:38:MET:HE2   | 1.71                     | 0.54              |
| 1:A:382:PHE:C    | 1:A:382:PHE:CD2  | 2.81                     | 0.54              |
| 1:D:370:THR:HG23 | 1:D:421:ILE:O    | 2.07                     | 0.54              |
| 1:S:105:ASP:HB3  | 1:X:297:MET:HE1  | 1.86                     | 0.54              |
| 1:A:407:ILE:O    | 1:A:411:ALA:HB2  | 2.08                     | 0.54              |
| 1:W:362:THR:HG22 | 1:W:362:THR:O    | 2.07                     | 0.54              |
| 1:W:18:ILE:HG22  | 1:W:344:ILE:HG12 | 1.89                     | 0.54              |
| 1:U:55:MET:HA    | 1:U:331:VAL:HG13 | 1.89                     | 0.54              |
| 2:G:46:PHE:HB3   | 2:G:95:LEU:HD21  | 1.89                     | 0.54              |
| 2:P:8:ARG:O      | 2:P:9:ASN:HB2    | 2.06                     | 0.54              |
| 1:B:352:LEU:O    | 1:B:355:GLN:HB2  | 2.07                     | 0.54              |
| 2:L:89:ARG:O     | 2:L:90:LYS:CB    | 2.55                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:344:ILE:CG2  | 3:X:461:ATP:C2   | 2.90                     | 0.54              |
| 1:T:37:ARG:NH1   | 1:T:37:ARG:HG2   | 2.22                     | 0.54              |
| 1:W:349:HIS:O    | 1:W:350:ALA:HB3  | 2.07                     | 0.54              |
| 1:T:5:THR:OG1    | 1:T:6:PRO:HD2    | 2.06                     | 0.54              |
| 2:R:49:GLY:O     | 2:R:50:THR:C     | 2.46                     | 0.54              |
| 1:X:68:ARG:HG3   | 1:X:68:ARG:HH11  | 1.72                     | 0.54              |
| 1:U:283:LEU:HB3  | 1:U:284:PRO:HD3  | 1.89                     | 0.54              |
| 1:S:233:LYS:C    | 1:S:235:ILE:N    | 2.59                     | 0.54              |
| 1:C:6:PRO:HD3    | 1:C:32:ARG:HG2   | 1.90                     | 0.54              |
| 2:K:1:THR:CG2    | 2:K:33:LYS:HD3   | 2.37                     | 0.54              |
| 1:X:245:ILE:CG2  | 1:X:249:GLU:HG3  | 2.37                     | 0.54              |
| 1:D:280:ARG:HA   | 1:D:283:LEU:HD12 | 1.89                     | 0.54              |
| 1:B:34:ARG:CZ    | 1:B:251:ASN:HA   | 2.38                     | 0.54              |
| 1:E:378:ALA:O    | 1:E:379:GLU:C    | 2.46                     | 0.54              |
| 1:C:245:ILE:O    | 1:C:246:ASP:C    | 2.46                     | 0.54              |
| 1:U:349:HIS:O    | 1:U:350:ALA:HB3  | 2.08                     | 0.54              |
| 2:M:49:GLY:O     | 2:M:50:THR:C     | 2.44                     | 0.54              |
| 2:N:104:LEU:HD13 | 2:N:112:VAL:CG1  | 2.38                     | 0.54              |
| 1:T:235:ILE:HG22 | 1:T:236:ASN:N    | 2.23                     | 0.54              |
| 1:T:333:LEU:N    | 1:T:333:LEU:HD23 | 2.23                     | 0.54              |
| 1:T:63:LYS:N     | 3:T:457:ATP:O2B  | 2.35                     | 0.54              |
| 1:B:241:LYS:HG2  | 1:B:295:HIS:ND1  | 2.22                     | 0.54              |
| 1:B:370:THR:O    | 1:B:373:ALA:HB3  | 2.08                     | 0.54              |
| 1:F:13:LEU:HD13  | 1:F:24:LYS:HG2   | 1.90                     | 0.54              |
| 1:X:333:LEU:HD23 | 1:X:333:LEU:N    | 2.23                     | 0.54              |
| 1:U:96:VAL:HG11  | 1:U:281:ASP:O    | 2.08                     | 0.54              |
| 1:W:5:THR:OG1    | 1:W:6:PRO:HD2    | 2.08                     | 0.54              |
| 1:X:236:ASN:N    | 1:X:237:PRO:HD3  | 2.21                     | 0.54              |
| 1:D:9:ILE:HD13   | 1:D:31:LEU:HD23  | 1.88                     | 0.54              |
| 1:U:120:ARG:HG3  | 1:U:232:ALA:HB2  | 1.89                     | 0.54              |
| 2:K:38:TYR:CD1   | 2:K:69:GLY:HA3   | 2.42                     | 0.54              |
| 1:B:250:GLN:HA   | 1:B:250:GLN:HE21 | 1.72                     | 0.54              |
| 1:D:360:MET:HE2  | 1:D:360:MET:N    | 2.23                     | 0.54              |
| 1:W:98:SER:HA    | 1:W:101:ARG:NH1  | 2.23                     | 0.54              |
| 1:E:384:VAL:O    | 1:E:385:ASN:C    | 2.46                     | 0.54              |
| 1:E:398:THR:HG22 | 1:E:399:VAL:N    | 2.22                     | 0.54              |
| 1:U:100:ILE:HG13 | 1:U:291:VAL:HG21 | 1.89                     | 0.54              |
| 2:G:61:GLU:O     | 2:G:62:ARG:C     | 2.46                     | 0.54              |
| 1:U:20:GLN:OE1   | 1:U:333:LEU:HB3  | 2.08                     | 0.54              |
| 2:Q:105:ILE:HG22 | 2:Q:113:VAL:O    | 2.07                     | 0.54              |
| 1:B:409:PHE:CE1  | 1:C:6:PRO:HB3    | 2.41                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:443:ILE:HG12 | 2:G:112:VAL:CG2  | 2.38                     | 0.54              |
| 1:W:315:ARG:HB3  | 1:W:316:PRO:HD2  | 1.90                     | 0.54              |
| 1:X:80:LYS:HG3   | 1:X:255:PHE:HD2  | 1.72                     | 0.54              |
| 2:N:128:ASN:HA   | 2:N:131:LEU:HB3  | 1.90                     | 0.54              |
| 1:E:17:ILE:HD12  | 1:E:17:ILE:N     | 2.22                     | 0.54              |
| 1:F:275:ARG:C    | 1:F:277:GLY:N    | 2.58                     | 0.54              |
| 1:U:120:ARG:HH12 | 1:U:234:LEU:HB3  | 1.72                     | 0.54              |
| 1:C:347:GLU:HB2  | 1:C:348:PRO:HD3  | 1.89                     | 0.54              |
| 1:F:316:PRO:C    | 1:F:318:ASP:H    | 2.11                     | 0.54              |
| 2:H:4:VAL:HG22   | 2:H:5:SER:N      | 2.22                     | 0.54              |
| 1:T:68:ARG:HH11  | 1:T:68:ARG:HG3   | 1.73                     | 0.54              |
| 2:H:52:ASP:CA    | 2:H:55:THR:HG23  | 2.35                     | 0.54              |
| 1:A:235:ILE:HG22 | 1:A:236:ASN:N    | 2.23                     | 0.54              |
| 1:U:437:GLU:OE2  | 1:U:439:LEU:HG   | 2.08                     | 0.54              |
| 1:B:283:LEU:O    | 1:B:287:GLU:HB2  | 2.06                     | 0.54              |
| 1:S:341:PHE:O    | 1:S:345:LEU:HB2  | 2.08                     | 0.54              |
| 1:W:112:ARG:HG2  | 1:W:112:ARG:O    | 2.08                     | 0.54              |
| 1:T:441:ARG:HH11 | 1:T:441:ARG:HG3  | 1.72                     | 0.54              |
| 1:A:6:PRO:HB3    | 1:F:409:PHE:HD1  | 1.69                     | 0.54              |
| 2:J:17:ASP:CG    | 2:J:163:THR:HG23 | 2.28                     | 0.54              |
| 1:T:54:LEU:HD21  | 1:T:327:LEU:HD22 | 1.90                     | 0.54              |
| 1:E:283:LEU:CB   | 1:E:284:PRO:HD3  | 2.37                     | 0.54              |
| 1:D:16:HIS:C     | 1:D:17:ILE:HD12  | 2.28                     | 0.54              |
| 1:F:20:GLN:H     | 1:F:20:GLN:HE21  | 1.55                     | 0.54              |
| 1:B:37:ARG:CG    | 1:B:38:MET:N     | 2.71                     | 0.54              |
| 2:O:55:THR:HG22  | 2:P:83:ARG:CG    | 2.37                     | 0.54              |
| 2:H:98:ALA:HB2   | 2:H:103:SER:HA   | 1.90                     | 0.54              |
| 1:U:311:PHE:HE1  | 1:U:316:PRO:HA   | 1.73                     | 0.54              |
| 1:B:61:VAL:HA    | 1:B:336:LEU:HD22 | 1.89                     | 0.54              |
| 2:G:42:VAL:HG12  | 2:G:99:ASP:HB3   | 1.89                     | 0.54              |
| 1:S:370:THR:HG23 | 1:S:373:ALA:HB3  | 1.90                     | 0.54              |
| 1:F:433:VAL:HG12 | 1:F:434:VAL:N    | 2.17                     | 0.54              |
| 2:P:1:THR:HG23   | 2:P:33:LYS:HD3   | 1.90                     | 0.54              |
| 1:X:37:ARG:NH1   | 1:X:37:ARG:HG2   | 2.22                     | 0.54              |
| 1:E:37:ARG:HH12  | 1:E:38:MET:HE2   | 1.72                     | 0.54              |
| 1:A:227:ILE:HG23 | 1:A:228:ASP:H    | 1.72                     | 0.54              |
| 1:B:300:THR:HA   | 1:B:303:ILE:HG12 | 1.90                     | 0.54              |
| 1:X:98:SER:HA    | 1:X:101:ARG:NH1  | 2.23                     | 0.54              |
| 1:D:113:GLN:HG2  | 1:D:113:GLN:O    | 2.08                     | 0.54              |
| 1:W:313:VAL:CG2  | 1:W:314:ALA:H    | 2.02                     | 0.53              |
| 1:W:63:LYS:NZ    | 3:W:460:ATP:O2G  | 2.41                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:283:LEU:HB3  | 1:W:284:PRO:HD3  | 1.90                     | 0.53              |
| 1:T:426:VAL:O    | 1:T:429:ALA:HB3  | 2.07                     | 0.53              |
| 1:C:341:PHE:O    | 1:C:345:LEU:HB2  | 2.08                     | 0.53              |
| 1:C:440:SER:O    | 1:C:442:PHE:N    | 2.41                     | 0.53              |
| 1:V:370:THR:HG23 | 1:V:373:ALA:HB3  | 1.89                     | 0.53              |
| 1:A:250:GLN:NE2  | 1:A:250:GLN:HA   | 2.23                     | 0.53              |
| 1:A:38:MET:HG3   | 1:A:45:ARG:NH1   | 2.23                     | 0.53              |
| 1:D:262:ILE:O    | 1:D:262:ILE:HG13 | 2.07                     | 0.53              |
| 1:C:367:ILE:HD11 | 1:C:421:ILE:HD11 | 1.89                     | 0.53              |
| 1:B:13:LEU:CD1   | 1:B:24:LYS:HG2   | 2.38                     | 0.53              |
| 1:C:56:ILE:N     | 1:C:56:ILE:CD1   | 2.71                     | 0.53              |
| 1:C:34:ARG:CZ    | 1:C:251:ASN:HA   | 2.39                     | 0.53              |
| 1:T:362:THR:HG22 | 1:T:362:THR:O    | 2.08                     | 0.53              |
| 1:E:326:ARG:O    | 1:E:328:PRO:HD3  | 2.09                     | 0.53              |
| 1:T:63:LYS:HZ2   | 1:T:63:LYS:HB2   | 1.73                     | 0.53              |
| 2:G:137:LEU:N    | 2:G:137:LEU:CD1  | 2.71                     | 0.53              |
| 2:L:17:ASP:HB2   | 2:L:164:ASN:HD22 | 1.68                     | 0.53              |
| 2:N:107:THR:OG1  | 2:N:111:ASP:OD2  | 2.21                     | 0.53              |
| 1:S:260:ASP:HB3  | 1:S:311:PHE:CE2  | 2.43                     | 0.53              |
| 1:E:71:ALA:HB1   | 1:E:78:PHE:HB2   | 1.89                     | 0.53              |
| 1:A:382:PHE:C    | 1:A:382:PHE:HD2  | 2.11                     | 0.53              |
| 1:E:275:ARG:O    | 1:E:277:GLY:N    | 2.41                     | 0.53              |
| 1:E:377:ILE:O    | 1:E:380:ALA:HB3  | 2.09                     | 0.53              |
| 2:K:42:VAL:HG12  | 2:K:99:ASP:HB3   | 1.90                     | 0.53              |
| 1:D:41:GLN:HE21  | 1:D:41:GLN:CA    | 2.21                     | 0.53              |
| 2:Q:55:THR:O     | 2:Q:59:LEU:HB2   | 2.08                     | 0.53              |
| 2:N:56:LEU:CD2   | 2:N:95:LEU:HD13  | 2.39                     | 0.53              |
| 1:C:20:GLN:CA    | 1:C:20:GLN:NE2   | 2.71                     | 0.53              |
| 1:E:77:PRO:HD2   | 1:E:251:ASN:O    | 2.09                     | 0.53              |
| 1:C:316:PRO:C    | 1:C:318:ASP:H    | 2.12                     | 0.53              |
| 1:V:236:ASN:HD21 | 1:V:239:GLU:HB3  | 1.73                     | 0.53              |
| 2:J:165:THR:HA   | 2:J:167:PHE:CE2  | 2.44                     | 0.53              |
| 1:S:437:GLU:HG3  | 1:S:440:SER:HB2  | 1.89                     | 0.53              |
| 1:F:341:PHE:HA   | 1:F:344:ILE:CG1  | 2.38                     | 0.53              |
| 1:T:17:ILE:HD13  | 1:T:66:ILE:HG12  | 1.91                     | 0.53              |
| 1:A:409:PHE:O    | 1:B:6:PRO:HG2    | 2.09                     | 0.53              |
| 2:R:17:ASP:HB2   | 2:R:164:ASN:HD21 | 1.72                     | 0.53              |
| 1:S:311:PHE:HE1  | 1:S:316:PRO:HA   | 1.73                     | 0.53              |
| 1:T:96:VAL:CG1   | 1:T:282:LEU:HD12 | 2.37                     | 0.53              |
| 1:D:37:ARG:HG2   | 1:D:38:MET:N     | 2.23                     | 0.53              |
| 1:F:5:THR:OG1    | 1:F:8:GLU:HB2    | 2.08                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:341:PHE:O    | 1:X:345:LEU:HB2  | 2.08                     | 0.53              |
| 1:F:12:GLU:O     | 1:F:15:GLN:HB2   | 2.09                     | 0.53              |
| 1:D:3:GLU:HG3    | 1:D:4:MET:N      | 2.22                     | 0.53              |
| 1:B:5:THR:O      | 1:B:9:ILE:HG13   | 2.08                     | 0.53              |
| 1:F:37:ARG:NH1   | 1:F:38:MET:HE2   | 2.23                     | 0.53              |
| 1:U:370:THR:CG2  | 1:U:422:ASP:HA   | 2.38                     | 0.53              |
| 2:I:144:SER:HB3  | 2:I:147:GLU:CG   | 2.35                     | 0.53              |
| 1:D:17:ILE:CD1   | 1:D:17:ILE:N     | 2.69                     | 0.53              |
| 1:U:442:PHE:O    | 1:U:443:ILE:HD13 | 2.08                     | 0.53              |
| 1:V:20:GLN:OE1   | 1:V:333:LEU:HB3  | 2.08                     | 0.53              |
| 1:S:98:SER:HA    | 1:S:101:ARG:NH1  | 2.24                     | 0.53              |
| 1:E:316:PRO:C    | 1:E:318:ASP:H    | 2.12                     | 0.53              |
| 1:V:315:ARG:HB3  | 1:V:316:PRO:HD2  | 1.91                     | 0.53              |
| 1:W:55:MET:HA    | 1:W:331:VAL:HG13 | 1.90                     | 0.53              |
| 1:U:60:GLY:HA3   | 1:U:392:GLY:HA3  | 1.90                     | 0.53              |
| 1:X:353:THR:HG22 | 1:X:369:PHE:CD1  | 2.43                     | 0.53              |
| 1:F:37:ARG:HG2   | 1:F:38:MET:N     | 2.22                     | 0.53              |
| 2:H:82:TRP:CZ2   | 2:H:91:LEU:HD13  | 2.35                     | 0.53              |
| 1:D:37:ARG:HH22  | 1:D:250:GLN:HE22 | 1.55                     | 0.53              |
| 1:E:380:ALA:O    | 1:E:383:ARG:HB3  | 2.09                     | 0.53              |
| 2:G:85:ASP:N     | 2:G:85:ASP:OD2   | 2.39                     | 0.53              |
| 1:C:20:GLN:NE2   | 1:C:20:GLN:HA    | 2.24                     | 0.53              |
| 1:C:55:MET:CE    | 1:C:306:ILE:HG21 | 2.39                     | 0.53              |
| 1:A:76:ALA:HB1   | 1:A:251:ASN:O    | 2.08                     | 0.53              |
| 2:I:67:HIS:CD2   | 2:I:73:LYS:HD3   | 2.44                     | 0.53              |
| 2:H:165:THR:HA   | 2:H:167:PHE:CE2  | 2.44                     | 0.53              |
| 1:A:398:THR:HG22 | 1:A:399:VAL:N    | 2.22                     | 0.53              |
| 1:U:68:ARG:HG3   | 1:U:68:ARG:HH11  | 1.73                     | 0.53              |
| 1:V:259:ILE:O    | 1:V:262:ILE:HG12 | 2.08                     | 0.53              |
| 1:X:283:LEU:HD11 | 1:X:322:GLU:HB3  | 1.90                     | 0.53              |
| 1:W:17:ILE:HD13  | 1:W:66:ILE:HG12  | 1.89                     | 0.53              |
| 2:H:83:ARG:HG3   | 2:I:55:THR:HG22  | 1.90                     | 0.53              |
| 1:S:18:ILE:HG22  | 1:S:344:ILE:CG1  | 2.39                     | 0.53              |
| 2:R:164:ASN:HD22 | 2:R:164:ASN:N    | 1.97                     | 0.53              |
| 1:C:341:PHE:HA   | 1:C:344:ILE:CG1  | 2.38                     | 0.53              |
| 2:L:1:THR:CG2    | 2:L:33:LYS:HD3   | 2.39                     | 0.53              |
| 2:M:55:THR:HG22  | 2:N:83:ARG:CB    | 2.38                     | 0.53              |
| 1:C:104:THR:O    | 1:C:107:ALA:HB3  | 2.07                     | 0.53              |
| 1:X:5:THR:OG1    | 1:X:6:PRO:HD2    | 2.07                     | 0.53              |
| 1:U:120:ARG:NE   | 1:U:232:ALA:HA   | 2.23                     | 0.53              |
| 2:M:83:ARG:HB3   | 2:R:55:THR:HG22  | 1.91                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:108:MET:O    | 1:C:109:LYS:C    | 2.46                     | 0.53              |
| 2:K:161:VAL:HG22 | 2:P:24:ASN:O     | 2.09                     | 0.53              |
| 1:F:105:ASP:OD1  | 1:F:294:LYS:HE2  | 2.09                     | 0.53              |
| 1:V:437:GLU:HG2  | 1:V:437:GLU:O    | 2.09                     | 0.53              |
| 1:E:322:GLU:N    | 1:E:322:GLU:OE2  | 2.37                     | 0.53              |
| 1:T:65:GLU:HG2   | 3:T:457:ATP:H5'2 | 1.90                     | 0.53              |
| 1:S:369:PHE:CE2  | 1:S:421:ILE:HD12 | 2.32                     | 0.53              |
| 2:N:4:VAL:HG12   | 2:N:153:LEU:HD21 | 1.91                     | 0.53              |
| 1:T:370:THR:CG2  | 1:T:422:ASP:HA   | 2.39                     | 0.53              |
| 1:U:369:PHE:CE2  | 1:U:421:ILE:HD12 | 2.34                     | 0.53              |
| 1:E:293:THR:C    | 1:E:295:HIS:H    | 2.11                     | 0.53              |
| 1:A:104:THR:OG1  | 1:A:293:THR:HG21 | 2.08                     | 0.53              |
| 2:P:55:THR:HG22  | 2:Q:83:ARG:CB    | 2.38                     | 0.53              |
| 1:F:54:LEU:HG    | 1:F:56:ILE:HD11  | 1.91                     | 0.53              |
| 1:U:48:VAL:HG23  | 1:V:355:GLN:OE1  | 2.08                     | 0.53              |
| 1:S:120:ARG:HD2  | 1:S:120:ARG:C    | 2.29                     | 0.53              |
| 1:S:444:LEU:HD13 | 1:S:444:LEU:H    | 1.73                     | 0.53              |
| 2:O:95:LEU:O     | 2:O:105:ILE:HA   | 2.09                     | 0.53              |
| 1:A:57:GLY:CA    | 1:A:63:LYS:HE3   | 2.38                     | 0.53              |
| 2:G:1:THR:HG22   | 2:G:2:THR:H      | 1.74                     | 0.53              |
| 2:I:164:ASN:HD22 | 2:I:164:ASN:C    | 2.11                     | 0.53              |
| 1:F:37:ARG:HA    | 1:F:40:LEU:CD1   | 2.38                     | 0.53              |
| 2:P:8:ARG:HH11   | 2:P:8:ARG:CB     | 2.16                     | 0.53              |
| 1:V:441:ARG:HG3  | 1:V:441:ARG:HH11 | 1.73                     | 0.53              |
| 2:I:137:LEU:HD11 | 2:O:136:ALA:HB1  | 1.91                     | 0.53              |
| 1:C:37:ARG:CG    | 1:C:38:MET:N     | 2.72                     | 0.53              |
| 1:U:235:ILE:CG2  | 1:U:236:ASN:N    | 2.72                     | 0.53              |
| 1:E:56:ILE:HD12  | 1:E:56:ILE:N     | 2.24                     | 0.53              |
| 2:L:165:THR:HA   | 2:L:167:PHE:CE2  | 2.43                     | 0.53              |
| 2:P:127:GLY:O    | 2:P:129:TYR:N    | 2.41                     | 0.53              |
| 1:S:283:LEU:HB3  | 1:S:284:PRO:HD3  | 1.90                     | 0.53              |
| 1:B:264:LYS:O    | 1:B:265:LYS:HB3  | 2.09                     | 0.53              |
| 1:F:441:ARG:NH2  | 2:G:37:LEU:HD23  | 2.24                     | 0.53              |
| 1:S:426:VAL:O    | 1:S:429:ALA:HB3  | 2.09                     | 0.53              |
| 2:O:104:LEU:HD13 | 2:O:112:VAL:CG1  | 2.39                     | 0.53              |
| 1:F:443:ILE:HG21 | 2:L:114:GLN:HG3  | 1.90                     | 0.53              |
| 1:E:262:ILE:HD12 | 1:E:278:VAL:HB   | 1.91                     | 0.53              |
| 1:A:249:GLU:HG2  | 1:A:299:LYS:H    | 1.74                     | 0.53              |
| 1:S:356:TYR:OH   | 1:X:51:LYS:HE2   | 2.08                     | 0.53              |
| 1:S:26:ALA:HA    | 1:S:29:ILE:HG12  | 1.91                     | 0.53              |
| 1:U:333:LEU:HD23 | 1:U:333:LEU:N    | 2.24                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:56:LEU:CD2   | 2:R:95:LEU:HD22  | 2.38                     | 0.52              |
| 2:I:88:LEU:O     | 2:I:89:ARG:C     | 2.47                     | 0.52              |
| 1:W:370:THR:CG2  | 1:W:422:ASP:HA   | 2.38                     | 0.52              |
| 1:B:366:ASN:O    | 1:B:418:THR:HA   | 2.09                     | 0.52              |
| 1:W:286:VAL:HA   | 1:W:305:PHE:CE1  | 2.43                     | 0.52              |
| 1:D:347:GLU:N    | 1:D:348:PRO:CD   | 2.71                     | 0.52              |
| 1:B:403:LEU:CD1  | 1:B:426:VAL:HG22 | 2.39                     | 0.52              |
| 1:B:404:MET:O    | 1:B:408:SER:HB2  | 2.10                     | 0.52              |
| 1:X:369:PHE:CE2  | 1:X:421:ILE:HD12 | 2.33                     | 0.52              |
| 1:U:353:THR:HG22 | 1:U:369:PHE:CD1  | 2.44                     | 0.52              |
| 1:B:378:ALA:O    | 1:B:379:GLU:C    | 2.44                     | 0.52              |
| 2:H:1:THR:HG23   | 2:H:33:LYS:HD3   | 1.91                     | 0.52              |
| 2:H:1:THR:HG22   | 2:H:2:THR:N      | 2.24                     | 0.52              |
| 2:I:105:ILE:HG22 | 2:I:113:VAL:O    | 2.09                     | 0.52              |
| 1:W:260:ASP:HB3  | 1:W:311:PHE:CE2  | 2.43                     | 0.52              |
| 1:S:315:ARG:HB3  | 1:S:316:PRO:HD2  | 1.90                     | 0.52              |
| 1:C:62:GLY:O     | 1:C:63:LYS:C     | 2.46                     | 0.52              |
| 1:S:61:VAL:HA    | 1:S:336:LEU:HD21 | 1.92                     | 0.52              |
| 1:U:111:VAL:CG1  | 1:U:240:LEU:HD11 | 2.39                     | 0.52              |
| 1:B:343:ARG:C    | 1:B:345:LEU:N    | 2.62                     | 0.52              |
| 1:B:280:ARG:HH11 | 1:B:280:ARG:HG3  | 1.74                     | 0.52              |
| 2:M:4:VAL:HG12   | 2:M:153:LEU:HD21 | 1.91                     | 0.52              |
| 1:B:357:LYS:HA   | 1:B:367:ILE:CG2  | 2.40                     | 0.52              |
| 1:B:370:THR:O    | 1:B:373:ALA:N    | 2.40                     | 0.52              |
| 1:A:119:ASN:HB3  | 1:A:234:LEU:CD1  | 2.39                     | 0.52              |
| 1:X:315:ARG:HB3  | 1:X:316:PRO:HD2  | 1.91                     | 0.52              |
| 1:E:54:LEU:HG    | 1:E:56:ILE:CD1   | 2.39                     | 0.52              |
| 1:C:381:ALA:HB2  | 1:C:396:LEU:HD23 | 1.91                     | 0.52              |
| 1:T:18:ILE:HG22  | 1:T:344:ILE:HG12 | 1.90                     | 0.52              |
| 1:W:430:LEU:HG   | 1:W:431:GLY:H    | 1.73                     | 0.52              |
| 2:M:56:LEU:HD21  | 2:M:95:LEU:HB2   | 1.90                     | 0.52              |
| 1:X:439:LEU:O    | 1:X:441:ARG:N    | 2.43                     | 0.52              |
| 2:I:91:LEU:O     | 2:I:108:GLY:HA3  | 2.10                     | 0.52              |
| 2:H:46:PHE:HB3   | 2:H:95:LEU:HD21  | 1.91                     | 0.52              |
| 1:S:355:GLN:OE1  | 1:X:48:VAL:HG23  | 2.10                     | 0.52              |
| 2:K:18:GLY:N     | 2:K:164:ASN:HD21 | 2.03                     | 0.52              |
| 1:B:51:LYS:O     | 1:B:52:ASN:O     | 2.27                     | 0.52              |
| 1:E:249:GLU:HG2  | 1:E:299:LYS:H    | 1.75                     | 0.52              |
| 2:H:43:LEU:O     | 2:H:97:VAL:HA    | 2.09                     | 0.52              |
| 1:V:349:HIS:O    | 1:V:350:ALA:HB3  | 2.08                     | 0.52              |
| 1:U:362:THR:O    | 1:U:362:THR:HG22 | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:403:LEU:CD2  | 1:F:404:MET:SD   | 2.97                     | 0.52              |
| 2:R:7:ARG:NH1    | 2:R:12:VAL:CG2   | 2.73                     | 0.52              |
| 1:S:422:ASP:O    | 1:S:426:VAL:HG23 | 2.09                     | 0.52              |
| 2:G:77:GLU:O     | 2:G:80:LYS:HG2   | 2.09                     | 0.52              |
| 1:T:260:ASP:HB3  | 1:T:311:PHE:CE2  | 2.44                     | 0.52              |
| 1:X:20:GLN:HB3   | 1:X:23:ALA:HB3   | 1.91                     | 0.52              |
| 1:V:353:THR:HG22 | 1:V:369:PHE:CD1  | 2.43                     | 0.52              |
| 1:D:38:MET:HG3   | 1:D:45:ARG:NH1   | 2.24                     | 0.52              |
| 1:V:96:VAL:CG1   | 1:V:282:LEU:HD12 | 2.38                     | 0.52              |
| 1:X:260:ASP:HB3  | 1:X:311:PHE:CE2  | 2.43                     | 0.52              |
| 1:A:101:ARG:HA   | 1:A:293:THR:HG22 | 1.90                     | 0.52              |
| 1:D:382:PHE:C    | 1:D:382:PHE:HD2  | 2.13                     | 0.52              |
| 2:R:157:GLY:HA2  | 2:R:163:THR:HG22 | 1.92                     | 0.52              |
| 2:H:128:ASN:O    | 2:H:131:LEU:HB3  | 2.10                     | 0.52              |
| 1:S:404:MET:HA   | 1:S:407:ILE:HG22 | 1.92                     | 0.52              |
| 2:Q:127:GLY:O    | 2:Q:129:TYR:N    | 2.42                     | 0.52              |
| 2:Q:89:ARG:HH11  | 2:R:87:ALA:HB2   | 1.73                     | 0.52              |
| 1:S:313:VAL:CG2  | 1:S:314:ALA:H    | 2.02                     | 0.52              |
| 1:A:360:MET:HA   | 1:A:360:MET:CE   | 2.40                     | 0.52              |
| 1:X:370:THR:CG2  | 1:X:422:ASP:HA   | 2.38                     | 0.52              |
| 1:S:359:LEU:HD11 | 1:X:48:VAL:HG21  | 1.90                     | 0.52              |
| 1:A:233:LYS:HD2  | 1:A:234:LEU:HB2  | 1.91                     | 0.52              |
| 1:V:96:VAL:HG11  | 1:V:281:ASP:O    | 2.09                     | 0.52              |
| 1:S:16:HIS:HA    | 1:S:348:PRO:HB3  | 1.92                     | 0.52              |
| 1:V:34:ARG:HG2   | 1:V:250:GLN:HE21 | 1.75                     | 0.52              |
| 2:P:157:GLY:HA2  | 2:P:163:THR:HG22 | 1.91                     | 0.52              |
| 2:R:95:LEU:O     | 2:R:105:ILE:HA   | 2.10                     | 0.52              |
| 2:P:95:LEU:O     | 2:P:105:ILE:HA   | 2.10                     | 0.52              |
| 2:M:8:ARG:O      | 2:M:9:ASN:HB2    | 2.08                     | 0.52              |
| 1:B:382:PHE:CD2  | 1:B:382:PHE:C    | 2.83                     | 0.52              |
| 1:V:54:LEU:HD21  | 1:V:327:LEU:HD22 | 1.91                     | 0.52              |
| 2:P:128:ASN:HA   | 2:P:131:LEU:HB3  | 1.92                     | 0.52              |
| 1:S:247:ALA:O    | 1:S:251:ASN:N    | 2.37                     | 0.52              |
| 1:A:370:THR:O    | 1:A:373:ALA:HB3  | 2.09                     | 0.52              |
| 2:R:55:THR:O     | 2:R:59:LEU:HB2   | 2.09                     | 0.52              |
| 1:X:100:ILE:HG13 | 1:X:291:VAL:HG21 | 1.92                     | 0.52              |
| 1:T:26:ALA:HA    | 1:T:29:ILE:HG12  | 1.91                     | 0.52              |
| 2:K:3:ILE:HG22   | 2:K:96:ILE:HD12  | 1.90                     | 0.52              |
| 2:N:49:GLY:O     | 2:N:50:THR:C     | 2.47                     | 0.52              |
| 1:A:264:LYS:HD3  | 1:A:276:GLU:CD   | 2.30                     | 0.52              |
| 1:F:403:LEU:HD22 | 1:F:404:MET:HG2  | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:56:LEU:CD2   | 2:M:95:LEU:HD22  | 2.40                     | 0.52              |
| 2:M:118:ASP:O    | 2:M:120:ILE:N    | 2.43                     | 0.52              |
| 1:X:96:VAL:CG1   | 1:X:282:LEU:HD12 | 2.39                     | 0.52              |
| 1:D:347:GLU:HB2  | 1:D:348:PRO:HD3  | 1.91                     | 0.52              |
| 1:D:55:MET:HE3   | 1:D:306:ILE:HG21 | 1.92                     | 0.52              |
| 1:W:333:LEU:N    | 1:W:333:LEU:HD23 | 2.25                     | 0.52              |
| 1:A:360:MET:HE3  | 1:B:36:ARG:NH1   | 2.24                     | 0.52              |
| 1:W:322:GLU:HG3  | 1:X:394:ARG:HH12 | 1.74                     | 0.52              |
| 1:A:439:LEU:HA   | 1:A:443:ILE:HD12 | 1.91                     | 0.52              |
| 1:T:421:ILE:O    | 1:T:421:ILE:HG22 | 2.09                     | 0.52              |
| 1:S:344:ILE:CG2  | 3:S:456:ATP:C2   | 2.93                     | 0.52              |
| 1:S:17:ILE:HD13  | 1:S:66:ILE:HG12  | 1.92                     | 0.52              |
| 1:U:422:ASP:O    | 1:U:426:VAL:HG23 | 2.10                     | 0.52              |
| 1:E:337:SER:OG   | 1:E:338:ALA:N    | 2.42                     | 0.52              |
| 2:N:49:GLY:O     | 2:N:51:ALA:N     | 2.43                     | 0.52              |
| 1:T:437:GLU:O    | 1:T:439:LEU:HD23 | 2.09                     | 0.52              |
| 1:S:63:LYS:HB2   | 3:S:456:ATP:O2B  | 2.10                     | 0.52              |
| 1:F:6:PRO:HD3    | 1:F:32:ARG:HG2   | 1.92                     | 0.52              |
| 1:A:54:LEU:HG    | 1:A:56:ILE:CD1   | 2.40                     | 0.52              |
| 1:W:26:ALA:HA    | 1:W:29:ILE:HG12  | 1.92                     | 0.52              |
| 1:C:101:ARG:HA   | 1:C:293:THR:HG22 | 1.91                     | 0.52              |
| 1:W:34:ARG:HG2   | 1:W:250:GLN:HE21 | 1.74                     | 0.52              |
| 1:V:98:SER:HA    | 1:V:101:ARG:NH1  | 2.24                     | 0.52              |
| 2:L:7:ARG:CZ     | 2:L:12:VAL:HG22  | 2.39                     | 0.52              |
| 1:A:276:GLU:HG2  | 1:A:276:GLU:O    | 2.11                     | 0.51              |
| 2:M:7:ARG:NH1    | 2:M:12:VAL:CG2   | 2.73                     | 0.51              |
| 1:W:20:GLN:OE1   | 1:W:333:LEU:HB3  | 2.10                     | 0.51              |
| 1:X:48:VAL:HG13  | 1:X:48:VAL:O     | 2.10                     | 0.51              |
| 1:V:370:THR:HG23 | 1:V:373:ALA:CB   | 2.40                     | 0.51              |
| 1:E:79:ILE:CG2   | 1:E:103:LEU:HD13 | 2.37                     | 0.51              |
| 1:E:83:ALA:HB1   | 1:E:262:ILE:HD13 | 1.92                     | 0.51              |
| 1:D:415:ASN:OD1  | 1:D:416:GLY:N    | 2.42                     | 0.51              |
| 2:L:71:LEU:HD13  | 2:L:71:LEU:C     | 2.30                     | 0.51              |
| 2:I:115:PRO:CB   | 2:I:119:GLN:HA   | 2.41                     | 0.51              |
| 1:B:57:GLY:HA3   | 1:B:63:LYS:HE3   | 1.91                     | 0.51              |
| 1:C:406:LYS:HD2  | 1:C:406:LYS:N    | 2.13                     | 0.51              |
| 2:R:120:ILE:O    | 2:R:121:LEU:HD23 | 2.11                     | 0.51              |
| 1:S:96:VAL:HG11  | 1:S:281:ASP:O    | 2.09                     | 0.51              |
| 1:E:250:GLN:HA   | 1:E:250:GLN:NE2  | 2.25                     | 0.51              |
| 1:F:280:ARG:HG3  | 1:F:280:ARG:NH1  | 2.25                     | 0.51              |
| 1:T:115:GLU:C    | 1:T:117:ALA:H    | 2.12                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:55:THR:O     | 2:N:59:LEU:HB2   | 2.09                     | 0.51              |
| 1:E:381:ALA:HB2  | 1:E:396:LEU:HD23 | 1.92                     | 0.51              |
| 1:V:108:MET:SD   | 1:V:244:ALA:CB   | 2.97                     | 0.51              |
| 1:F:338:ALA:N    | 1:F:382:PHE:HD1  | 2.08                     | 0.51              |
| 1:A:360:MET:N    | 1:A:360:MET:HE2  | 2.25                     | 0.51              |
| 2:Q:5:SER:CB     | 2:Q:14:VAL:HG22  | 2.38                     | 0.51              |
| 2:N:120:ILE:O    | 2:N:121:LEU:HD23 | 2.10                     | 0.51              |
| 2:I:1:THR:HG22   | 2:I:2:THR:N      | 2.25                     | 0.51              |
| 1:F:65:GLU:O     | 1:F:66:ILE:C     | 2.48                     | 0.51              |
| 2:M:83:ARG:CG    | 2:R:55:THR:HG22  | 2.39                     | 0.51              |
| 1:T:48:VAL:HG23  | 1:U:355:GLN:OE1  | 2.10                     | 0.51              |
| 1:F:384:VAL:O    | 1:F:385:ASN:C    | 2.48                     | 0.51              |
| 1:U:80:LYS:HG3   | 1:U:255:PHE:HD2  | 1.73                     | 0.51              |
| 2:R:105:ILE:HG22 | 2:R:113:VAL:O    | 2.11                     | 0.51              |
| 1:F:33:ASN:HA    | 1:F:36:ARG:HD2   | 1.91                     | 0.51              |
| 2:R:133:ALA:O    | 2:R:136:ALA:HB3  | 2.10                     | 0.51              |
| 1:W:370:THR:HG23 | 1:W:373:ALA:HB3  | 1.92                     | 0.51              |
| 1:X:422:ASP:O    | 1:X:426:VAL:HG23 | 2.10                     | 0.51              |
| 2:M:55:THR:O     | 2:M:59:LEU:HB2   | 2.11                     | 0.51              |
| 1:X:9:ILE:HD13   | 1:X:31:LEU:HD23  | 1.92                     | 0.51              |
| 1:U:120:ARG:HG3  | 1:U:232:ALA:HA   | 1.93                     | 0.51              |
| 1:F:293:THR:C    | 1:F:295:HIS:H    | 2.14                     | 0.51              |
| 2:K:82:TRP:CE2   | 2:K:88:LEU:HD13  | 2.45                     | 0.51              |
| 1:A:304:LEU:HD12 | 1:A:305:PHE:N    | 2.26                     | 0.51              |
| 2:L:115:PRO:HG3  | 2:L:121:LEU:HD11 | 1.92                     | 0.51              |
| 2:J:82:TRP:CE3   | 2:J:110:GLY:HA2  | 2.45                     | 0.51              |
| 1:U:315:ARG:HB3  | 1:U:316:PRO:CD   | 2.41                     | 0.51              |
| 2:O:105:ILE:HG22 | 2:O:113:VAL:O    | 2.10                     | 0.51              |
| 2:K:1:THR:HG23   | 2:K:33:LYS:CE    | 2.41                     | 0.51              |
| 1:T:96:VAL:HG11  | 1:T:281:ASP:O    | 2.10                     | 0.51              |
| 1:A:338:ALA:N    | 1:A:382:PHE:HD1  | 2.08                     | 0.51              |
| 1:E:382:PHE:CD2  | 1:E:382:PHE:C    | 2.83                     | 0.51              |
| 2:O:55:THR:O     | 2:O:59:LEU:HB2   | 2.11                     | 0.51              |
| 1:B:41:GLN:HE21  | 1:B:41:GLN:HA    | 1.75                     | 0.51              |
| 2:L:6:VAL:HG22   | 2:L:120:ILE:HG23 | 1.93                     | 0.51              |
| 1:U:430:LEU:HG   | 1:U:431:GLY:H    | 1.76                     | 0.51              |
| 1:E:107:ALA:O    | 1:E:111:VAL:HG23 | 2.11                     | 0.51              |
| 1:S:54:LEU:HD21  | 1:S:327:LEU:HD22 | 1.93                     | 0.51              |
| 2:O:164:ASN:HD22 | 2:O:164:ASN:N    | 1.98                     | 0.51              |
| 1:E:101:ARG:HA   | 1:E:293:THR:HG22 | 1.93                     | 0.51              |
| 1:C:377:ILE:O    | 1:C:380:ALA:HB3  | 2.11                     | 0.51              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:250:GLN:CA   | 1:B:250:GLN:HE21 | 2.21                     | 0.51              |
| 2:H:161:VAL:HG22 | 2:M:24:ASN:O     | 2.10                     | 0.51              |
| 2:R:56:LEU:HD23  | 2:R:95:LEU:HD13  | 1.93                     | 0.51              |
| 1:E:403:LEU:CD2  | 1:E:404:MET:N    | 2.72                     | 0.51              |
| 2:K:83:ARG:HG2   | 2:L:55:THR:CB    | 2.41                     | 0.51              |
| 1:W:369:PHE:HE2  | 1:W:421:ILE:CD1  | 2.20                     | 0.51              |
| 1:C:382:PHE:CD2  | 1:C:382:PHE:C    | 2.84                     | 0.51              |
| 1:D:34:ARG:NH2   | 1:D:253:ILE:HD13 | 2.25                     | 0.51              |
| 1:S:244:ALA:O    | 1:S:247:ALA:HB3  | 2.10                     | 0.51              |
| 1:C:347:GLU:N    | 1:C:348:PRO:CD   | 2.74                     | 0.51              |
| 1:T:324:GLN:HE22 | 1:U:389:GLU:HG2  | 1.75                     | 0.51              |
| 2:I:7:ARG:NH2    | 2:I:102:GLU:O    | 2.44                     | 0.51              |
| 2:R:37:LEU:HD22  | 2:R:61:GLU:HG3   | 1.93                     | 0.51              |
| 1:V:311:PHE:HE1  | 1:V:316:PRO:HA   | 1.75                     | 0.51              |
| 1:F:37:ARG:CG    | 1:F:38:MET:N     | 2.74                     | 0.51              |
| 1:C:337:SER:OG   | 1:C:338:ALA:N    | 2.43                     | 0.51              |
| 1:A:337:SER:OG   | 1:A:338:ALA:N    | 2.43                     | 0.51              |
| 2:Q:1:THR:HG23   | 2:Q:33:LYS:HD3   | 1.92                     | 0.51              |
| 2:H:116:GLU:HG2  | 2:I:30:ASN:ND2   | 2.26                     | 0.51              |
| 2:M:56:LEU:CD2   | 2:M:95:LEU:HD13  | 2.41                     | 0.51              |
| 2:N:90:LYS:O     | 2:N:91:LEU:HD12  | 2.11                     | 0.51              |
| 1:E:356:TYR:HE1  | 1:E:400:MET:HB3  | 1.75                     | 0.51              |
| 1:X:303:ILE:HG22 | 1:X:304:LEU:N    | 2.23                     | 0.51              |
| 1:D:34:ARG:CZ    | 1:D:251:ASN:HA   | 2.41                     | 0.51              |
| 1:D:78:PHE:CG    | 1:D:79:ILE:N     | 2.78                     | 0.51              |
| 2:I:46:PHE:HB3   | 2:I:95:LEU:HD23  | 1.92                     | 0.51              |
| 1:T:112:ARG:O    | 1:T:116:ILE:HB   | 2.10                     | 0.51              |
| 1:V:20:GLN:HB3   | 1:V:23:ALA:HB3   | 1.92                     | 0.51              |
| 1:X:434:VAL:O    | 1:X:435:GLU:O    | 2.29                     | 0.51              |
| 2:J:61:GLU:O     | 2:J:62:ARG:C     | 2.46                     | 0.51              |
| 1:T:34:ARG:HG2   | 1:T:250:GLN:HE21 | 1.76                     | 0.51              |
| 1:B:381:ALA:O    | 1:B:384:VAL:HG13 | 2.11                     | 0.51              |
| 1:S:439:LEU:CD2  | 1:S:439:LEU:H    | 2.21                     | 0.51              |
| 1:W:65:GLU:HG2   | 3:W:460:ATP:C5'  | 2.29                     | 0.51              |
| 1:S:357:LYS:CA   | 1:S:367:ILE:HD11 | 2.32                     | 0.51              |
| 2:N:33:LYS:HA    | 2:N:46:PHE:CZ    | 2.46                     | 0.51              |
| 1:T:370:THR:HG23 | 1:T:373:ALA:HB3  | 1.93                     | 0.51              |
| 1:B:378:ALA:O    | 1:B:380:ALA:N    | 2.44                     | 0.51              |
| 1:F:58:PRO:O     | 1:F:63:LYS:NZ    | 2.41                     | 0.51              |
| 1:D:116:ILE:CD1  | 1:D:117:ALA:N    | 2.74                     | 0.51              |
| 1:V:441:ARG:O    | 1:V:443:ILE:N    | 2.44                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:63:LYS:HB2   | 1:V:63:LYS:HZ2   | 1.76                     | 0.51              |
| 1:D:111:VAL:HG21 | 1:D:244:ALA:CA   | 2.41                     | 0.51              |
| 1:D:44:LEU:HA    | 1:D:47:GLU:HB2   | 1.93                     | 0.51              |
| 1:F:407:ILE:O    | 1:F:411:ALA:HB2  | 2.11                     | 0.51              |
| 1:E:52:ASN:ND2   | 1:E:305:PHE:CB   | 2.72                     | 0.50              |
| 1:W:353:THR:HG22 | 1:W:369:PHE:CD1  | 2.46                     | 0.50              |
| 1:C:439:LEU:HD23 | 1:C:443:ILE:HD12 | 1.93                     | 0.50              |
| 2:M:37:LEU:HD22  | 2:M:61:GLU:HG3   | 1.94                     | 0.50              |
| 1:S:96:VAL:HG21  | 1:S:281:ASP:HB3  | 1.93                     | 0.50              |
| 1:D:439:LEU:HD23 | 2:J:72:LEU:HG    | 1.91                     | 0.50              |
| 1:A:283:LEU:CB   | 1:A:284:PRO:HD3  | 2.42                     | 0.50              |
| 1:F:54:LEU:HG    | 1:F:56:ILE:CD1   | 2.41                     | 0.50              |
| 1:U:45:ARG:O     | 1:U:48:VAL:HG12  | 2.11                     | 0.50              |
| 1:F:403:LEU:CD2  | 1:F:404:MET:N    | 2.71                     | 0.50              |
| 1:S:21:ALA:C     | 1:S:23:ALA:N     | 2.64                     | 0.50              |
| 1:A:233:LYS:HD2  | 1:A:233:LYS:C    | 2.32                     | 0.50              |
| 1:V:96:VAL:HG21  | 1:V:281:ASP:HB3  | 1.94                     | 0.50              |
| 2:P:112:VAL:HB   | 1:V:443:ILE:CD1  | 2.42                     | 0.50              |
| 1:F:69:ARG:O     | 1:F:70:LEU:C     | 2.50                     | 0.50              |
| 1:T:336:LEU:HB2  | 1:T:341:PHE:HE1  | 1.75                     | 0.50              |
| 1:W:48:VAL:HG13  | 1:W:48:VAL:O     | 2.12                     | 0.50              |
| 1:F:31:LEU:CD2   | 1:F:74:ALA:HB2   | 2.41                     | 0.50              |
| 1:B:71:ALA:HB1   | 1:B:78:PHE:HB2   | 1.92                     | 0.50              |
| 1:F:119:ASN:ND2  | 1:F:235:ILE:N    | 2.58                     | 0.50              |
| 2:P:92:GLU:O     | 2:P:93:ALA:HB2   | 2.12                     | 0.50              |
| 1:C:12:GLU:O     | 1:C:15:GLN:HB2   | 2.11                     | 0.50              |
| 1:F:341:PHE:HA   | 1:F:344:ILE:HG12 | 1.94                     | 0.50              |
| 1:B:403:LEU:HD12 | 1:B:426:VAL:HG22 | 1.94                     | 0.50              |
| 1:E:33:ASN:HA    | 1:E:36:ARG:HD2   | 1.91                     | 0.50              |
| 2:H:57:PHE:HA    | 2:H:95:LEU:HD11  | 1.92                     | 0.50              |
| 1:W:54:LEU:HD21  | 1:W:327:LEU:HD22 | 1.93                     | 0.50              |
| 2:H:55:THR:HG21  | 2:H:89:ARG:HH21  | 1.77                     | 0.50              |
| 1:U:370:THR:HG23 | 1:U:373:ALA:HB3  | 1.92                     | 0.50              |
| 1:X:96:VAL:HG11  | 1:X:281:ASP:O    | 2.12                     | 0.50              |
| 1:D:443:ILE:HD11 | 2:J:72:LEU:HD11  | 1.92                     | 0.50              |
| 1:F:366:ASN:O    | 1:F:418:THR:HA   | 2.10                     | 0.50              |
| 1:X:336:LEU:HB2  | 1:X:341:PHE:HE1  | 1.76                     | 0.50              |
| 1:V:280:ARG:HH22 | 1:W:261:LYS:HE3  | 1.75                     | 0.50              |
| 1:S:34:ARG:HG2   | 1:S:250:GLN:HE21 | 1.75                     | 0.50              |
| 1:U:26:ALA:HA    | 1:U:29:ILE:HG12  | 1.92                     | 0.50              |
| 1:U:34:ARG:HG2   | 1:U:250:GLN:HE21 | 1.76                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:49:GLY:O     | 2:O:50:THR:C     | 2.49                     | 0.50              |
| 2:Q:76:VAL:HG22  | 1:W:443:ILE:HD11 | 1.93                     | 0.50              |
| 1:E:264:LYS:HE3  | 1:E:264:LYS:H    | 1.73                     | 0.50              |
| 2:R:83:ARG:HH12  | 1:X:442:PHE:HB2  | 1.76                     | 0.50              |
| 2:N:95:LEU:O     | 2:N:105:ILE:HA   | 2.12                     | 0.50              |
| 1:S:370:THR:HG23 | 1:S:373:ALA:CB   | 2.41                     | 0.50              |
| 2:R:134:ALA:O    | 2:R:137:LEU:N    | 2.45                     | 0.50              |
| 1:B:337:SER:OG   | 1:B:338:ALA:N    | 2.43                     | 0.50              |
| 2:L:1:THR:HG23   | 2:L:33:LYS:HD3   | 1.94                     | 0.50              |
| 1:W:315:ARG:HB3  | 1:W:316:PRO:CD   | 2.41                     | 0.50              |
| 1:F:107:ALA:HB2  | 1:F:248:VAL:HG23 | 1.94                     | 0.50              |
| 1:E:79:ILE:HD12  | 1:E:80:LYS:H     | 1.75                     | 0.50              |
| 1:D:262:ILE:HD12 | 1:D:278:VAL:HB   | 1.94                     | 0.50              |
| 1:V:107:ALA:O    | 1:V:111:VAL:HG23 | 2.12                     | 0.50              |
| 1:V:236:ASN:ND2  | 1:V:239:GLU:HB3  | 2.27                     | 0.50              |
| 1:T:45:ARG:O     | 1:T:48:VAL:HG12  | 2.11                     | 0.50              |
| 1:T:48:VAL:O     | 1:T:48:VAL:HG13  | 2.12                     | 0.50              |
| 1:X:34:ARG:HG2   | 1:X:250:GLN:HE21 | 1.76                     | 0.50              |
| 1:W:404:MET:HA   | 1:W:407:ILE:HG22 | 1.93                     | 0.50              |
| 1:S:100:ILE:HG13 | 1:S:291:VAL:HG21 | 1.93                     | 0.50              |
| 2:O:1:THR:HG23   | 2:O:33:LYS:HD3   | 1.93                     | 0.50              |
| 1:W:245:ILE:HG22 | 1:W:249:GLU:HG3  | 1.94                     | 0.50              |
| 2:Q:7:ARG:NH1    | 2:Q:12:VAL:CG2   | 2.75                     | 0.50              |
| 1:U:279:GLN:O    | 1:U:320:ILE:HD11 | 2.11                     | 0.50              |
| 1:U:260:ASP:HB3  | 1:U:311:PHE:CE2  | 2.46                     | 0.50              |
| 2:Q:95:LEU:O     | 2:Q:105:ILE:HA   | 2.11                     | 0.50              |
| 1:S:20:GLN:HB3   | 1:S:23:ALA:HB3   | 1.93                     | 0.50              |
| 2:L:17:ASP:OD2   | 2:L:33:LYS:HE3   | 2.11                     | 0.50              |
| 2:O:37:LEU:HD22  | 2:O:61:GLU:HG3   | 1.93                     | 0.50              |
| 1:W:96:VAL:HG11  | 1:W:281:ASP:O    | 2.10                     | 0.50              |
| 1:C:403:LEU:HD22 | 1:C:404:MET:HG2  | 1.94                     | 0.50              |
| 1:D:337:SER:OG   | 1:D:338:ALA:N    | 2.44                     | 0.50              |
| 2:N:55:THR:HG22  | 2:O:83:ARG:CG    | 2.42                     | 0.50              |
| 1:B:41:GLN:HE21  | 1:B:41:GLN:CA    | 2.24                     | 0.50              |
| 1:F:119:ASN:HD21 | 1:F:235:ILE:N    | 2.09                     | 0.50              |
| 1:C:73:LEU:C     | 1:C:73:LEU:HD12  | 2.32                     | 0.50              |
| 1:B:374:VAL:O    | 1:B:375:LYS:C    | 2.50                     | 0.50              |
| 1:W:63:LYS:HZ2   | 1:W:63:LYS:HB2   | 1.77                     | 0.50              |
| 1:W:357:LYS:HA   | 1:W:367:ILE:CD1  | 2.32                     | 0.50              |
| 1:W:421:ILE:O    | 1:W:421:ILE:HG22 | 2.11                     | 0.50              |
| 1:X:370:THR:HG23 | 1:X:373:ALA:HB3  | 1.93                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:236:ASN:ND2  | 1:A:239:GLU:CB   | 2.73                     | 0.50              |
| 1:C:439:LEU:HA   | 1:C:443:ILE:CD1  | 2.38                     | 0.50              |
| 1:X:18:ILE:HG22  | 1:X:344:ILE:HG12 | 1.94                     | 0.50              |
| 1:V:426:VAL:O    | 1:V:429:ALA:HB3  | 2.12                     | 0.50              |
| 1:D:20:GLN:CA    | 1:D:20:GLN:HE21  | 2.24                     | 0.50              |
| 1:W:96:VAL:HG21  | 1:W:281:ASP:HB3  | 1.94                     | 0.50              |
| 1:S:363:GLU:OE1  | 1:X:32:ARG:NH2   | 2.40                     | 0.50              |
| 2:P:133:ALA:O    | 2:P:136:ALA:HB3  | 2.11                     | 0.50              |
| 1:B:38:MET:HG3   | 1:B:45:ARG:NH1   | 2.26                     | 0.50              |
| 1:S:236:ASN:HB3  | 1:S:239:GLU:CB   | 2.41                     | 0.50              |
| 1:V:404:MET:HA   | 1:V:407:ILE:HG22 | 1.94                     | 0.50              |
| 1:F:249:GLU:HG2  | 1:F:299:LYS:H    | 1.77                     | 0.50              |
| 2:R:37:LEU:HD23  | 1:S:441:ARG:NH2  | 2.26                     | 0.50              |
| 1:U:344:ILE:HG23 | 3:U:458:ATP:C2   | 2.44                     | 0.50              |
| 1:T:315:ARG:HB3  | 1:T:316:PRO:CD   | 2.41                     | 0.50              |
| 1:V:422:ASP:O    | 1:V:426:VAL:HG23 | 2.12                     | 0.50              |
| 2:O:5:SER:CB     | 2:O:14:VAL:HG22  | 2.40                     | 0.50              |
| 1:X:311:PHE:HE1  | 1:X:316:PRO:HA   | 1.77                     | 0.50              |
| 1:A:44:LEU:O     | 1:A:48:VAL:HG12  | 2.12                     | 0.50              |
| 1:E:37:ARG:HH22  | 1:E:250:GLN:HE22 | 1.59                     | 0.50              |
| 2:Q:37:LEU:HD22  | 2:Q:61:GLU:HG3   | 1.93                     | 0.50              |
| 2:P:7:ARG:NH1    | 2:P:12:VAL:CG2   | 2.75                     | 0.50              |
| 2:N:151:LYS:O    | 2:N:155:ILE:HD13 | 2.12                     | 0.50              |
| 1:E:20:GLN:H     | 1:E:20:GLN:HE21  | 1.60                     | 0.50              |
| 1:T:422:ASP:O    | 1:T:426:VAL:HG23 | 2.11                     | 0.50              |
| 1:W:422:ASP:O    | 1:W:426:VAL:HG23 | 2.11                     | 0.50              |
| 2:H:78:LEU:HD11  | 2:H:82:TRP:HZ3   | 1.76                     | 0.50              |
| 2:H:6:VAL:HG12   | 2:H:7:ARG:N      | 2.26                     | 0.50              |
| 2:P:37:LEU:HD22  | 2:P:61:GLU:HG3   | 1.94                     | 0.50              |
| 2:O:7:ARG:NH1    | 2:O:12:VAL:CG2   | 2.75                     | 0.50              |
| 1:E:65:GLU:HG3   | 3:E:454:ATP:H2'  | 1.92                     | 0.50              |
| 2:J:137:LEU:HD13 | 2:P:136:ALA:HB1  | 1.92                     | 0.50              |
| 1:B:44:LEU:HA    | 1:B:47:GLU:HB2   | 1.93                     | 0.50              |
| 1:C:262:ILE:HD12 | 1:C:278:VAL:HB   | 1.93                     | 0.50              |
| 2:N:7:ARG:NH1    | 2:N:12:VAL:CG2   | 2.75                     | 0.50              |
| 2:L:56:LEU:C     | 2:L:56:LEU:CD2   | 2.80                     | 0.50              |
| 1:W:370:THR:HG23 | 1:W:373:ALA:CB   | 2.42                     | 0.50              |
| 1:T:311:PHE:HE1  | 1:T:316:PRO:HA   | 1.77                     | 0.50              |
| 1:X:393:ALA:HB3  | 3:X:461:ATP:H1'  | 1.93                     | 0.50              |
| 1:D:355:GLN:O    | 1:D:359:LEU:HD23 | 2.12                     | 0.50              |
| 1:C:357:LYS:HG2  | 1:C:367:ILE:HG23 | 1.94                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:384:VAL:O    | 1:C:385:ASN:C    | 2.49                     | 0.50              |
| 2:Q:49:GLY:O     | 2:Q:50:THR:C     | 2.50                     | 0.50              |
| 1:B:344:ILE:CG2  | 3:B:451:ATP:C2   | 2.95                     | 0.49              |
| 1:S:54:LEU:CD2   | 1:S:307:ALA:HB3  | 2.42                     | 0.49              |
| 2:H:164:ASN:H    | 2:H:164:ASN:HD22 | 1.60                     | 0.49              |
| 1:X:21:ALA:C     | 1:X:23:ALA:N     | 2.64                     | 0.49              |
| 2:J:105:ILE:O    | 2:J:105:ILE:HG23 | 2.11                     | 0.49              |
| 1:C:403:LEU:CD2  | 1:C:404:MET:N    | 2.75                     | 0.49              |
| 1:W:45:ARG:O     | 1:W:48:VAL:HG12  | 2.12                     | 0.49              |
| 1:C:330:ARG:NH1  | 1:C:330:ARG:HG3  | 2.27                     | 0.49              |
| 1:S:336:LEU:HB2  | 1:S:341:PHE:HE1  | 1.77                     | 0.49              |
| 2:G:25:THR:HA    | 2:R:159:ILE:O    | 2.11                     | 0.49              |
| 2:L:154:ARG:O    | 2:L:155:ILE:C    | 2.50                     | 0.49              |
| 1:T:100:ILE:HG13 | 1:T:291:VAL:HG21 | 1.93                     | 0.49              |
| 1:E:347:GLU:HB2  | 1:E:348:PRO:HD3  | 1.94                     | 0.49              |
| 1:F:73:LEU:C     | 1:F:73:LEU:HD12  | 2.33                     | 0.49              |
| 1:V:260:ASP:HB3  | 1:V:311:PHE:CE2  | 2.46                     | 0.49              |
| 2:J:1:THR:HG23   | 2:J:33:LYS:CE    | 2.41                     | 0.49              |
| 1:B:356:TYR:O    | 1:B:357:LYS:C    | 2.50                     | 0.49              |
| 1:B:378:ALA:C    | 1:B:380:ALA:N    | 2.63                     | 0.49              |
| 2:L:17:ASP:HB2   | 2:L:164:ASN:HD21 | 1.75                     | 0.49              |
| 1:T:431:GLY:O    | 1:T:432:GLU:HG3  | 2.12                     | 0.49              |
| 2:I:43:LEU:O     | 2:I:97:VAL:HA    | 2.11                     | 0.49              |
| 1:T:229:ASP:O    | 1:T:233:LYS:HG3  | 2.11                     | 0.49              |
| 1:D:264:LYS:HZ3  | 1:D:279:GLN:HE22 | 1.49                     | 0.49              |
| 2:K:137:LEU:O    | 2:K:141:THR:CG2  | 2.52                     | 0.49              |
| 1:S:369:PHE:HE2  | 1:S:421:ILE:CD1  | 2.21                     | 0.49              |
| 2:I:1:THR:HG23   | 2:I:33:LYS:CE    | 2.43                     | 0.49              |
| 1:U:426:VAL:O    | 1:U:429:ALA:HB3  | 2.12                     | 0.49              |
| 2:K:86:ARG:CG    | 2:K:87:ALA:H     | 2.22                     | 0.49              |
| 2:L:164:ASN:HD22 | 2:L:164:ASN:C    | 2.16                     | 0.49              |
| 1:W:260:ASP:HB3  | 1:W:311:PHE:HD2  | 1.73                     | 0.49              |
| 1:D:57:GLY:HA3   | 1:D:63:LYS:HE3   | 1.94                     | 0.49              |
| 1:C:387:LYS:HD2  | 1:C:435:GLU:OE1  | 2.13                     | 0.49              |
| 2:K:82:TRP:NE1   | 2:K:88:LEU:HB3   | 2.27                     | 0.49              |
| 1:F:235:ILE:HG22 | 1:F:237:PRO:HD3  | 1.95                     | 0.49              |
| 1:F:337:SER:OG   | 1:F:338:ALA:N    | 2.43                     | 0.49              |
| 1:U:63:LYS:HB2   | 1:U:63:LYS:HZ2   | 1.77                     | 0.49              |
| 1:B:310:ALA:O    | 1:B:311:PHE:HB2  | 2.10                     | 0.49              |
| 2:K:17:ASP:O     | 2:K:33:LYS:HD2   | 2.11                     | 0.49              |
| 1:F:57:GLY:CA    | 1:F:63:LYS:HE3   | 2.41                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:65:GLU:HG2   | 3:X:461:ATP:H5'2 | 1.94                     | 0.49              |
| 1:U:96:VAL:CG1   | 1:U:282:LEU:HD12 | 2.39                     | 0.49              |
| 1:F:360:MET:HA   | 1:F:360:MET:HE1  | 1.94                     | 0.49              |
| 2:O:133:ALA:O    | 2:O:136:ALA:HB3  | 2.12                     | 0.49              |
| 1:F:356:TYR:HE1  | 1:F:400:MET:HB3  | 1.76                     | 0.49              |
| 1:T:404:MET:HA   | 1:T:407:ILE:HG22 | 1.94                     | 0.49              |
| 1:E:257:ASP:OD1  | 1:E:308:SER:OG   | 2.31                     | 0.49              |
| 1:V:26:ALA:HA    | 1:V:29:ILE:HG12  | 1.94                     | 0.49              |
| 1:V:315:ARG:HB3  | 1:V:316:PRO:CD   | 2.42                     | 0.49              |
| 1:E:403:LEU:HD12 | 1:E:426:VAL:HG13 | 1.94                     | 0.49              |
| 1:E:407:ILE:HD11 | 1:E:425:TYR:OH   | 2.12                     | 0.49              |
| 2:N:4:VAL:HA     | 2:N:121:LEU:O    | 2.13                     | 0.49              |
| 1:A:440:SER:O    | 1:A:442:PHE:N    | 2.45                     | 0.49              |
| 1:T:369:PHE:HE2  | 1:T:421:ILE:CD1  | 2.21                     | 0.49              |
| 2:P:120:ILE:O    | 2:P:121:LEU:HD23 | 2.12                     | 0.49              |
| 1:U:441:ARG:O    | 1:U:443:ILE:N    | 2.44                     | 0.49              |
| 1:W:9:ILE:HD13   | 1:W:31:LEU:HD23  | 1.94                     | 0.49              |
| 2:L:151:LYS:O    | 2:L:155:ILE:HG13 | 2.13                     | 0.49              |
| 1:F:256:ILE:HG21 | 1:F:259:ILE:HD12 | 1.93                     | 0.49              |
| 1:T:245:ILE:HD11 | 1:T:295:HIS:HB3  | 1.93                     | 0.49              |
| 1:U:297:MET:HB2  | 1:V:109:LYS:NZ   | 2.28                     | 0.49              |
| 1:W:439:LEU:HG   | 1:W:440:SER:N    | 2.20                     | 0.49              |
| 1:U:55:MET:HE2   | 1:U:306:ILE:HG21 | 1.93                     | 0.49              |
| 1:E:402:ARG:O    | 1:E:405:ASP:HB2  | 2.13                     | 0.49              |
| 2:G:164:ASN:C    | 2:G:164:ASN:HD22 | 2.13                     | 0.49              |
| 1:C:382:PHE:C    | 1:C:382:PHE:HD2  | 2.16                     | 0.49              |
| 1:D:34:ARG:HH22  | 1:D:253:ILE:HD13 | 1.78                     | 0.49              |
| 1:U:120:ARG:NH1  | 1:U:234:LEU:HB3  | 2.28                     | 0.49              |
| 2:Q:118:ASP:OD1  | 2:Q:119:GLN:N    | 2.43                     | 0.49              |
| 1:F:382:PHE:O    | 1:F:383:ARG:C    | 2.50                     | 0.49              |
| 1:U:20:GLN:HB3   | 1:U:23:ALA:HB3   | 1.94                     | 0.49              |
| 1:U:21:ALA:C     | 1:U:23:ALA:N     | 2.65                     | 0.49              |
| 1:B:108:MET:HG3  | 1:B:295:HIS:CE1  | 2.48                     | 0.49              |
| 1:X:421:ILE:O    | 1:X:421:ILE:HG22 | 2.11                     | 0.49              |
| 2:J:83:ARG:HG2   | 2:K:55:THR:CG2   | 2.39                     | 0.49              |
| 1:U:9:ILE:HD13   | 1:U:31:LEU:HD23  | 1.94                     | 0.49              |
| 1:D:341:PHE:HA   | 1:D:344:ILE:CG1  | 2.42                     | 0.49              |
| 1:C:55:MET:C     | 1:C:56:ILE:HD12  | 2.32                     | 0.49              |
| 1:F:41:GLN:CA    | 1:F:41:GLN:HE21  | 2.26                     | 0.49              |
| 1:F:315:ARG:O    | 1:F:318:ASP:HB2  | 2.13                     | 0.49              |
| 2:J:107:THR:OG1  | 2:J:111:ASP:OD2  | 2.26                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:242:GLN:HA   | 1:F:242:GLN:OE1  | 2.12                     | 0.49              |
| 1:E:404:MET:O    | 1:E:408:SER:HB2  | 2.12                     | 0.49              |
| 2:G:36:ARG:NH1   | 2:G:170:GLU:OE2  | 2.46                     | 0.49              |
| 1:E:5:THR:OG1    | 1:E:8:GLU:HB2    | 2.12                     | 0.49              |
| 1:W:28:ALA:C     | 1:W:30:ALA:H     | 2.16                     | 0.49              |
| 1:U:404:MET:HA   | 1:U:407:ILE:HG22 | 1.95                     | 0.49              |
| 1:C:81:VAL:HG11  | 1:C:99:ILE:HG12  | 1.93                     | 0.49              |
| 1:A:113:GLN:HA   | 1:A:113:GLN:OE1  | 2.13                     | 0.49              |
| 1:W:65:GLU:CG    | 3:W:460:ATP:H5'2 | 2.26                     | 0.49              |
| 1:C:51:LYS:O     | 1:C:52:ASN:O     | 2.30                     | 0.49              |
| 1:V:444:LEU:C    | 1:V:444:LEU:HD23 | 2.32                     | 0.49              |
| 1:S:328:PRO:HB3  | 1:T:398:THR:HA   | 1.94                     | 0.49              |
| 2:G:137:LEU:O    | 2:G:141:THR:CG2  | 2.56                     | 0.49              |
| 1:V:45:ARG:O     | 1:V:48:VAL:HG12  | 2.12                     | 0.49              |
| 2:P:5:SER:CB     | 2:P:14:VAL:HG22  | 2.40                     | 0.49              |
| 1:D:20:GLN:HA    | 1:D:20:GLN:NE2   | 2.27                     | 0.49              |
| 3:E:454:ATP:C8   | 3:E:454:ATP:H5'1 | 2.48                     | 0.49              |
| 1:D:437:GLU:O    | 1:D:439:LEU:N    | 2.46                     | 0.49              |
| 2:O:55:THR:HG22  | 2:P:83:ARG:HB3   | 1.95                     | 0.49              |
| 1:B:236:ASN:C    | 1:B:238:GLU:H    | 2.16                     | 0.49              |
| 1:E:381:ALA:CB   | 1:E:396:LEU:HD23 | 2.42                     | 0.49              |
| 1:U:48:VAL:HG13  | 1:U:48:VAL:O     | 2.12                     | 0.49              |
| 1:A:341:PHE:O    | 1:A:345:LEU:HB2  | 2.12                     | 0.49              |
| 1:F:83:ALA:HB1   | 1:F:262:ILE:HD13 | 1.95                     | 0.49              |
| 1:A:264:LYS:HZ3  | 1:A:279:GLN:NE2  | 2.03                     | 0.49              |
| 1:T:55:MET:HE1   | 1:T:63:LYS:O     | 2.12                     | 0.49              |
| 1:U:370:THR:HG23 | 1:U:373:ALA:CB   | 2.43                     | 0.49              |
| 1:S:15:GLN:O     | 1:S:348:PRO:CA   | 2.61                     | 0.49              |
| 1:C:349:HIS:O    | 1:C:350:ALA:CB   | 2.59                     | 0.49              |
| 1:W:61:VAL:HA    | 1:W:336:LEU:HD21 | 1.94                     | 0.49              |
| 1:F:41:GLN:HE21  | 1:F:41:GLN:HA    | 1.77                     | 0.49              |
| 1:C:83:ALA:HB1   | 1:C:262:ILE:HD13 | 1.93                     | 0.49              |
| 2:H:120:ILE:HD11 | 2:H:138:VAL:HG21 | 1.95                     | 0.49              |
| 2:Q:104:LEU:HD13 | 2:Q:112:VAL:CG1  | 2.44                     | 0.48              |
| 2:I:79:ALA:CB    | 2:I:83:ARG:HH21  | 2.25                     | 0.48              |
| 1:V:322:GLU:HG3  | 1:W:394:ARG:HH12 | 1.78                     | 0.48              |
| 1:T:20:GLN:HB3   | 1:T:23:ALA:HB3   | 1.94                     | 0.48              |
| 1:E:443:ILE:HG21 | 2:K:114:GLN:HG3  | 1.94                     | 0.48              |
| 1:X:45:ARG:O     | 1:X:48:VAL:HG12  | 2.13                     | 0.48              |
| 1:S:315:ARG:HB3  | 1:S:316:PRO:CD   | 2.42                     | 0.48              |
| 1:D:444:LEU:HD21 | 2:K:20:VAL:HG21  | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:367:ILE:HD11 | 1:C:421:ILE:HD12 | 1.93                     | 0.48              |
| 1:B:38:MET:HA    | 1:B:45:ARG:HH11  | 1.78                     | 0.48              |
| 2:K:81:ASP:HB3   | 2:K:88:LEU:HD12  | 1.94                     | 0.48              |
| 2:Q:49:GLY:O     | 2:Q:51:ALA:N     | 2.45                     | 0.48              |
| 2:L:78:LEU:HD12  | 2:L:78:LEU:O     | 2.13                     | 0.48              |
| 1:W:55:MET:HE2   | 1:W:306:ILE:HG21 | 1.95                     | 0.48              |
| 2:L:137:LEU:O    | 2:L:141:THR:CG2  | 2.56                     | 0.48              |
| 1:C:444:LEU:HB3  | 2:I:113:VAL:HG22 | 1.95                     | 0.48              |
| 1:A:380:ALA:O    | 1:A:383:ARG:HB3  | 2.13                     | 0.48              |
| 1:C:41:GLN:HE21  | 1:C:41:GLN:CA    | 2.25                     | 0.48              |
| 1:W:28:ALA:O     | 1:W:30:ALA:N     | 2.46                     | 0.48              |
| 1:X:430:LEU:HG   | 1:X:431:GLY:H    | 1.78                     | 0.48              |
| 1:D:384:VAL:O    | 1:D:385:ASN:C    | 2.50                     | 0.48              |
| 2:G:7:ARG:NH2    | 2:G:102:GLU:O    | 2.46                     | 0.48              |
| 1:F:367:ILE:CD1  | 1:F:421:ILE:HD11 | 2.43                     | 0.48              |
| 1:W:20:GLN:HB3   | 1:W:23:ALA:HB3   | 1.93                     | 0.48              |
| 1:C:32:ARG:CZ    | 1:C:35:TRP:CE3   | 2.96                     | 0.48              |
| 2:L:17:ASP:CG    | 2:L:163:THR:HG23 | 2.33                     | 0.48              |
| 1:D:37:ARG:CG    | 1:D:38:MET:N     | 2.76                     | 0.48              |
| 1:D:240:LEU:O    | 1:D:243:LYS:N    | 2.45                     | 0.48              |
| 1:A:38:MET:HG3   | 1:A:45:ARG:HH12  | 1.77                     | 0.48              |
| 1:X:235:ILE:O    | 1:X:236:ASN:CB   | 2.60                     | 0.48              |
| 2:G:43:LEU:O     | 2:G:97:VAL:HA    | 2.14                     | 0.48              |
| 1:D:340:ASP:O    | 1:D:344:ILE:CD1  | 2.62                     | 0.48              |
| 1:X:112:ARG:CB   | 1:X:240:LEU:HD21 | 2.43                     | 0.48              |
| 1:T:120:ARG:HD2  | 1:T:120:ARG:O    | 2.13                     | 0.48              |
| 1:V:61:VAL:HA    | 1:V:336:LEU:HD21 | 1.95                     | 0.48              |
| 1:U:430:LEU:HD23 | 1:U:430:LEU:H    | 1.78                     | 0.48              |
| 1:X:430:LEU:H    | 1:X:430:LEU:HD23 | 1.78                     | 0.48              |
| 1:S:48:VAL:HG13  | 1:S:48:VAL:O     | 2.13                     | 0.48              |
| 1:A:403:LEU:CD2  | 1:A:404:MET:N    | 2.75                     | 0.48              |
| 2:O:90:LYS:O     | 2:O:91:LEU:HD12  | 2.14                     | 0.48              |
| 1:U:439:LEU:C    | 1:U:441:ARG:N    | 2.66                     | 0.48              |
| 1:F:275:ARG:O    | 1:F:278:VAL:HG23 | 2.14                     | 0.48              |
| 1:U:385:ASN:ND2  | 1:U:395:ARG:HE   | 2.08                     | 0.48              |
| 1:C:409:PHE:CE1  | 1:D:6:PRO:HB3    | 2.49                     | 0.48              |
| 1:C:250:GLN:HE21 | 1:C:250:GLN:HA   | 1.79                     | 0.48              |
| 2:I:38:TYR:CD1   | 2:I:69:GLY:HA3   | 2.48                     | 0.48              |
| 1:T:115:GLU:O    | 1:T:119:ASN:HB3  | 2.13                     | 0.48              |
| 2:I:67:HIS:HD2   | 2:I:73:LYS:HD3   | 1.78                     | 0.48              |
| 2:H:134:ALA:O    | 2:H:138:VAL:HG23 | 2.12                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:26:ALA:O     | 1:D:29:ILE:HG12  | 2.13                     | 0.48              |
| 1:B:410:SER:O    | 1:B:412:SER:N    | 2.46                     | 0.48              |
| 1:C:437:GLU:O    | 1:C:438:ASP:O    | 2.32                     | 0.48              |
| 1:A:85:LYS:O     | 1:A:85:LYS:HG2   | 2.12                     | 0.48              |
| 1:U:322:GLU:N    | 1:U:322:GLU:OE1  | 2.46                     | 0.48              |
| 1:C:17:ILE:HD12  | 1:C:17:ILE:N     | 2.29                     | 0.48              |
| 2:H:83:ARG:HG2   | 2:I:55:THR:CB    | 2.42                     | 0.48              |
| 2:H:91:LEU:N     | 2:H:91:LEU:CD1   | 2.71                     | 0.48              |
| 2:H:1:THR:HG23   | 2:H:33:LYS:HZ2   | 1.79                     | 0.48              |
| 1:W:311:PHE:HE1  | 1:W:316:PRO:HA   | 1.78                     | 0.48              |
| 1:W:15:GLN:O     | 1:W:349:HIS:N    | 2.41                     | 0.48              |
| 1:C:373:ALA:O    | 1:C:377:ILE:HG13 | 2.12                     | 0.48              |
| 1:B:436:ASN:HB3  | 1:B:439:LEU:CD1  | 2.44                     | 0.48              |
| 1:X:245:ILE:C    | 1:X:247:ALA:H    | 2.15                     | 0.48              |
| 1:V:61:VAL:HG11  | 1:V:335:ALA:HA   | 1.94                     | 0.48              |
| 1:A:227:ILE:HG23 | 1:A:228:ASP:N    | 2.28                     | 0.48              |
| 1:B:381:ALA:HB2  | 1:B:396:LEU:HD23 | 1.96                     | 0.48              |
| 2:K:131:LEU:O    | 2:K:132:SER:C    | 2.51                     | 0.48              |
| 2:Q:7:ARG:NE     | 2:Q:119:GLN:OE1  | 2.47                     | 0.48              |
| 1:F:381:ALA:HB2  | 1:F:396:LEU:HD23 | 1.95                     | 0.48              |
| 1:T:322:GLU:N    | 1:T:322:GLU:OE1  | 2.47                     | 0.48              |
| 1:W:322:GLU:OE1  | 1:W:322:GLU:N    | 2.46                     | 0.48              |
| 1:S:357:LYS:HA   | 1:S:367:ILE:CD1  | 2.31                     | 0.48              |
| 1:E:326:ARG:C    | 1:E:328:PRO:HD3  | 2.34                     | 0.48              |
| 2:P:56:LEU:CD2   | 2:P:95:LEU:HD13  | 2.43                     | 0.48              |
| 2:I:91:LEU:HD22  | 2:I:91:LEU:N     | 2.27                     | 0.48              |
| 1:A:6:PRO:HB3    | 1:F:409:PHE:CE1  | 2.45                     | 0.48              |
| 1:D:357:LYS:HE3  | 1:D:367:ILE:O    | 2.13                     | 0.48              |
| 2:P:112:VAL:HB   | 1:V:443:ILE:HD13 | 1.96                     | 0.48              |
| 2:L:6:VAL:HG12   | 2:L:7:ARG:N      | 2.28                     | 0.48              |
| 2:Q:20:VAL:HG21  | 1:X:444:LEU:HD21 | 1.95                     | 0.48              |
| 1:S:434:VAL:HG12 | 1:S:435:GLU:N    | 2.28                     | 0.48              |
| 1:B:263:CYS:SG   | 1:B:319:LEU:HD23 | 2.53                     | 0.48              |
| 1:F:23:ALA:CA    | 1:F:331:VAL:HG21 | 2.34                     | 0.48              |
| 2:M:4:VAL:HG12   | 2:M:153:LEU:CD2  | 2.44                     | 0.48              |
| 2:J:1:THR:HG23   | 2:J:33:LYS:HD3   | 1.94                     | 0.48              |
| 1:S:353:THR:HG22 | 1:S:369:PHE:HD1  | 1.79                     | 0.48              |
| 2:P:4:VAL:HG12   | 2:P:153:LEU:CD2  | 2.44                     | 0.48              |
| 2:H:88:LEU:C     | 2:H:90:LYS:N     | 2.64                     | 0.48              |
| 1:B:382:PHE:C    | 1:B:382:PHE:HD2  | 2.16                     | 0.48              |
| 2:H:164:ASN:H    | 2:H:164:ASN:ND2  | 2.12                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:240:LEU:O    | 1:D:241:LYS:C    | 2.52                     | 0.48              |
| 1:C:362:THR:HG23 | 1:D:39:GLN:HG2   | 1.95                     | 0.48              |
| 1:V:439:LEU:HD23 | 1:V:439:LEU:H    | 1.77                     | 0.48              |
| 1:S:385:ASN:ND2  | 1:S:395:ARG:HE   | 2.12                     | 0.48              |
| 1:B:436:ASN:O    | 1:B:437:GLU:C    | 2.52                     | 0.48              |
| 2:L:5:SER:HB2    | 2:L:14:VAL:HG22  | 1.95                     | 0.48              |
| 1:A:54:LEU:HD12  | 1:A:307:ALA:O    | 2.13                     | 0.48              |
| 1:U:101:ARG:HA   | 1:U:293:THR:HG22 | 1.96                     | 0.48              |
| 1:C:381:ALA:O    | 1:C:384:VAL:HG13 | 2.14                     | 0.48              |
| 1:X:26:ALA:HA    | 1:X:29:ILE:HG12  | 1.95                     | 0.48              |
| 2:K:141:THR:HG21 | 2:K:143:LEU:HD12 | 1.95                     | 0.48              |
| 2:J:1:THR:HG23   | 2:J:33:LYS:NZ    | 2.28                     | 0.48              |
| 2:R:4:VAL:HG12   | 2:R:153:LEU:HD21 | 1.96                     | 0.48              |
| 1:X:315:ARG:HB3  | 1:X:316:PRO:CD   | 2.44                     | 0.48              |
| 1:W:96:VAL:CG1   | 1:W:282:LEU:HD12 | 2.39                     | 0.48              |
| 2:I:46:PHE:HB3   | 2:I:95:LEU:HD21  | 1.95                     | 0.48              |
| 1:V:441:ARG:HG3  | 1:V:441:ARG:NH1  | 2.29                     | 0.48              |
| 1:U:336:LEU:HB2  | 1:U:341:PHE:HE1  | 1.79                     | 0.48              |
| 1:X:362:THR:HG22 | 1:X:362:THR:O    | 2.13                     | 0.48              |
| 1:B:56:ILE:CD1   | 1:B:56:ILE:N     | 2.76                     | 0.48              |
| 1:V:118:LYS:O    | 1:V:118:LYS:HG3  | 2.14                     | 0.48              |
| 1:B:440:SER:O    | 1:B:442:PHE:N    | 2.47                     | 0.48              |
| 1:D:433:VAL:HG22 | 1:D:434:VAL:N    | 2.29                     | 0.48              |
| 1:E:12:GLU:O     | 1:E:15:GLN:HB2   | 2.14                     | 0.48              |
| 2:M:7:ARG:NH1    | 2:M:12:VAL:HG21  | 2.29                     | 0.48              |
| 1:U:283:LEU:CD1  | 1:U:323:LEU:HD12 | 2.44                     | 0.48              |
| 1:W:21:ALA:C     | 1:W:23:ALA:N     | 2.67                     | 0.48              |
| 1:V:421:ILE:HG22 | 1:V:421:ILE:O    | 2.14                     | 0.48              |
| 1:A:262:ILE:HD12 | 1:A:278:VAL:HB   | 1.96                     | 0.48              |
| 1:B:435:GLU:HG2  | 1:B:436:ASN:H    | 1.79                     | 0.48              |
| 1:A:352:LEU:HD13 | 1:A:400:MET:CG   | 2.43                     | 0.48              |
| 1:C:55:MET:HE3   | 1:C:306:ILE:HG21 | 1.95                     | 0.48              |
| 1:X:404:MET:HA   | 1:X:407:ILE:HG22 | 1.95                     | 0.48              |
| 2:P:49:GLY:O     | 2:P:51:ALA:N     | 2.47                     | 0.48              |
| 1:C:34:ARG:HH22  | 1:C:253:ILE:HD13 | 1.79                     | 0.48              |
| 2:K:129:TYR:O    | 2:K:130:ALA:C    | 2.53                     | 0.48              |
| 1:A:403:LEU:HD22 | 1:A:404:MET:HG2  | 1.96                     | 0.48              |
| 2:H:83:ARG:CG    | 2:I:55:THR:HG22  | 2.44                     | 0.48              |
| 2:L:46:PHE:HB3   | 2:L:95:LEU:HD23  | 1.92                     | 0.48              |
| 2:G:105:ILE:O    | 2:G:105:ILE:HG23 | 2.14                     | 0.48              |
| 1:C:403:LEU:CD2  | 1:C:403:LEU:C    | 2.80                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:444:LEU:C    | 1:B:444:LEU:HD23 | 2.34                     | 0.48              |
| 1:C:111:VAL:HG12 | 1:C:112:ARG:N    | 2.29                     | 0.48              |
| 1:F:260:ASP:HB3  | 1:F:311:PHE:CE2  | 2.49                     | 0.48              |
| 1:W:100:ILE:HG13 | 1:W:291:VAL:HG21 | 1.95                     | 0.48              |
| 1:S:28:ALA:O     | 1:S:30:ALA:N     | 2.46                     | 0.48              |
| 2:P:151:LYS:O    | 2:P:155:ILE:HD13 | 2.13                     | 0.48              |
| 1:S:436:ASN:HD22 | 1:S:436:ASN:C    | 2.17                     | 0.48              |
| 2:J:18:GLY:H     | 2:J:164:ASN:ND2  | 2.01                     | 0.47              |
| 1:T:353:THR:HG22 | 1:T:369:PHE:HD1  | 1.78                     | 0.47              |
| 1:T:370:THR:HG23 | 1:T:373:ALA:CB   | 2.43                     | 0.47              |
| 1:W:426:VAL:O    | 1:W:429:ALA:HB3  | 2.13                     | 0.47              |
| 1:X:370:THR:HG23 | 1:X:373:ALA:CB   | 2.43                     | 0.47              |
| 1:F:17:ILE:N     | 1:F:17:ILE:CD1   | 2.72                     | 0.47              |
| 2:P:104:LEU:HD13 | 2:P:112:VAL:CG1  | 2.44                     | 0.47              |
| 1:B:439:LEU:CD2  | 2:H:72:LEU:HG    | 2.44                     | 0.47              |
| 1:A:20:GLN:CA    | 1:A:20:GLN:NE2   | 2.77                     | 0.47              |
| 1:X:61:VAL:HG11  | 1:X:335:ALA:HA   | 1.94                     | 0.47              |
| 1:X:336:LEU:HB2  | 1:X:341:PHE:CE1  | 2.49                     | 0.47              |
| 1:V:336:LEU:HB2  | 1:V:341:PHE:HE1  | 1.78                     | 0.47              |
| 1:C:278:VAL:O    | 1:C:281:ASP:HB2  | 2.14                     | 0.47              |
| 2:K:6:VAL:HG12   | 2:K:7:ARG:N      | 2.29                     | 0.47              |
| 1:C:44:LEU:HA    | 1:C:47:GLU:HB2   | 1.96                     | 0.47              |
| 2:Q:151:LYS:O    | 2:Q:155:ILE:HD13 | 2.14                     | 0.47              |
| 1:B:73:LEU:O     | 1:B:73:LEU:HD12  | 2.14                     | 0.47              |
| 2:J:82:TRP:HZ2   | 2:J:91:LEU:HD13  | 1.79                     | 0.47              |
| 1:U:60:GLY:N     | 3:U:458:ATP:O1B  | 2.47                     | 0.47              |
| 1:U:62:GLY:HA3   | 3:U:458:ATP:N7   | 2.29                     | 0.47              |
| 1:B:33:ASN:HA    | 1:B:36:ARG:HD2   | 1.96                     | 0.47              |
| 2:G:1:THR:HG23   | 2:G:33:LYS:HZ1   | 1.77                     | 0.47              |
| 2:Q:153:LEU:HB3  | 2:Q:167:PHE:CE2  | 2.49                     | 0.47              |
| 1:B:20:GLN:HE21  | 1:B:20:GLN:H     | 1.62                     | 0.47              |
| 1:E:358:ALA:HB1  | 1:F:40:LEU:HD22  | 1.97                     | 0.47              |
| 2:H:88:LEU:C     | 2:H:90:LYS:H     | 2.18                     | 0.47              |
| 1:U:421:ILE:O    | 1:U:421:ILE:HG22 | 2.13                     | 0.47              |
| 1:T:260:ASP:HB3  | 1:T:311:PHE:HD2  | 1.73                     | 0.47              |
| 1:T:96:VAL:HG21  | 1:T:281:ASP:HB3  | 1.95                     | 0.47              |
| 1:S:363:GLU:HG2  | 1:X:36:ARG:HH11  | 1.78                     | 0.47              |
| 1:S:362:THR:O    | 1:X:36:ARG:NH1   | 2.47                     | 0.47              |
| 1:C:38:MET:HG3   | 1:C:45:ARG:HH12  | 1.79                     | 0.47              |
| 1:U:120:ARG:HH21 | 1:U:235:ILE:HD13 | 1.79                     | 0.47              |
| 1:V:331:VAL:HG13 | 1:V:331:VAL:O    | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:70:HIS:O     | 2:H:71:LEU:C     | 2.51                     | 0.47              |
| 1:A:17:ILE:N     | 1:A:17:ILE:HD12  | 2.29                     | 0.47              |
| 1:E:112:ARG:O    | 1:E:114:GLN:N    | 2.47                     | 0.47              |
| 2:G:73:LYS:O     | 2:G:74:SER:C     | 2.53                     | 0.47              |
| 1:U:17:ILE:HD13  | 1:U:66:ILE:HG13  | 1.96                     | 0.47              |
| 1:T:357:LYS:HA   | 1:T:367:ILE:CD1  | 2.33                     | 0.47              |
| 1:E:403:LEU:C    | 1:E:405:ASP:H    | 2.17                     | 0.47              |
| 1:V:48:VAL:HG13  | 1:V:48:VAL:O     | 2.13                     | 0.47              |
| 1:E:37:ARG:CG    | 1:E:38:MET:N     | 2.76                     | 0.47              |
| 1:E:4:MET:HE2    | 1:E:9:ILE:HA     | 1.96                     | 0.47              |
| 1:A:65:GLU:HG3   | 3:A:450:ATP:H2'  | 1.95                     | 0.47              |
| 1:U:254:VAL:HB   | 1:U:305:PHE:CD2  | 2.48                     | 0.47              |
| 1:B:41:GLN:O     | 1:B:43:PRO:HD2   | 2.14                     | 0.47              |
| 1:C:262:ILE:O    | 1:C:262:ILE:HG13 | 2.13                     | 0.47              |
| 1:S:351:SER:OG   | 1:S:354:GLU:HG2  | 2.14                     | 0.47              |
| 1:S:444:LEU:H    | 1:S:444:LEU:CD1  | 2.28                     | 0.47              |
| 2:K:137:LEU:CD1  | 2:K:137:LEU:N    | 2.77                     | 0.47              |
| 1:S:421:ILE:O    | 1:S:421:ILE:HG22 | 2.13                     | 0.47              |
| 1:X:426:VAL:O    | 1:X:429:ALA:HB3  | 2.14                     | 0.47              |
| 1:W:54:LEU:CD2   | 1:W:307:ALA:HB3  | 2.44                     | 0.47              |
| 1:X:54:LEU:CD2   | 1:X:307:ALA:HB3  | 2.44                     | 0.47              |
| 1:F:64:THR:HB    | 3:F:455:ATP:O1A  | 2.14                     | 0.47              |
| 1:D:352:LEU:HD13 | 1:D:400:MET:CG   | 2.40                     | 0.47              |
| 1:B:275:ARG:O    | 1:B:277:GLY:N    | 2.47                     | 0.47              |
| 1:F:79:ILE:CG2   | 1:F:103:LEU:HD13 | 2.42                     | 0.47              |
| 1:E:409:PHE:CD2  | 1:F:25:ARG:NH2   | 2.83                     | 0.47              |
| 1:A:283:LEU:HD11 | 1:A:320:ILE:HD12 | 1.95                     | 0.47              |
| 1:T:336:LEU:HB2  | 1:T:341:PHE:CE1  | 2.50                     | 0.47              |
| 1:X:254:VAL:HB   | 1:X:305:PHE:CD2  | 2.49                     | 0.47              |
| 1:S:254:VAL:HB   | 1:S:305:PHE:CD2  | 2.49                     | 0.47              |
| 1:D:326:ARG:O    | 1:D:328:PRO:HD3  | 2.14                     | 0.47              |
| 1:F:283:LEU:O    | 1:F:284:PRO:C    | 2.53                     | 0.47              |
| 2:H:38:TYR:CD1   | 2:H:69:GLY:HA3   | 2.49                     | 0.47              |
| 1:A:13:LEU:HD13  | 1:A:24:LYS:HG2   | 1.96                     | 0.47              |
| 1:A:428:ASP:OD1  | 1:A:429:ALA:N    | 2.47                     | 0.47              |
| 1:D:441:ARG:NH2  | 2:K:61:GLU:OE2   | 2.48                     | 0.47              |
| 1:F:370:THR:O    | 1:F:371:THR:C    | 2.52                     | 0.47              |
| 1:B:264:LYS:NZ   | 1:B:318:ASP:O    | 2.45                     | 0.47              |
| 1:E:362:THR:HG23 | 1:F:39:GLN:HG2   | 1.97                     | 0.47              |
| 2:J:18:GLY:N     | 2:J:164:ASN:HD21 | 2.02                     | 0.47              |
| 2:Q:4:VAL:HA     | 2:Q:121:LEU:O    | 2.13                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:62:GLY:HA3   | 3:S:456:ATP:N7   | 2.28                     | 0.47              |
| 2:R:8:ARG:HH22   | 2:R:143:LEU:H    | 1.62                     | 0.47              |
| 1:U:54:LEU:CD2   | 1:U:307:ALA:HB3  | 2.44                     | 0.47              |
| 1:B:356:TYR:HE1  | 1:B:400:MET:HB3  | 1.79                     | 0.47              |
| 1:E:63:LYS:HB2   | 3:E:454:ATP:O2B  | 2.13                     | 0.47              |
| 2:G:88:LEU:O     | 2:G:89:ARG:HB2   | 2.13                     | 0.47              |
| 2:H:98:ALA:CB    | 2:H:103:SER:HA   | 2.45                     | 0.47              |
| 1:W:254:VAL:HB   | 1:W:305:PHE:CD2  | 2.50                     | 0.47              |
| 1:S:236:ASN:HB3  | 1:S:239:GLU:HB3  | 1.95                     | 0.47              |
| 1:A:4:MET:HE2    | 1:A:9:ILE:HA     | 1.96                     | 0.47              |
| 1:D:118:LYS:O    | 1:D:118:LYS:HD2  | 2.14                     | 0.47              |
| 1:A:264:LYS:NZ   | 1:A:319:LEU:HA   | 2.30                     | 0.47              |
| 1:V:260:ASP:HB3  | 1:V:311:PHE:HD2  | 1.73                     | 0.47              |
| 2:O:56:LEU:HD23  | 2:O:95:LEU:HD13  | 1.96                     | 0.47              |
| 1:V:9:ILE:HD13   | 1:V:31:LEU:HD23  | 1.96                     | 0.47              |
| 1:V:17:ILE:HG22  | 1:V:17:ILE:O     | 2.14                     | 0.47              |
| 1:U:297:MET:HB2  | 1:V:109:LYS:CE   | 2.45                     | 0.47              |
| 2:L:51:ALA:O     | 2:L:54:PHE:N     | 2.47                     | 0.47              |
| 2:R:127:GLY:O    | 2:R:129:TYR:N    | 2.48                     | 0.47              |
| 1:V:273:VAL:HG12 | 1:V:273:VAL:O    | 2.15                     | 0.47              |
| 1:F:330:ARG:HH11 | 1:F:330:ARG:HG3  | 1.79                     | 0.47              |
| 2:I:7:ARG:CZ     | 2:I:12:VAL:HG22  | 2.44                     | 0.47              |
| 1:V:322:GLU:N    | 1:V:322:GLU:OE1  | 2.48                     | 0.47              |
| 1:W:63:LYS:CB    | 3:W:460:ATP:O2B  | 2.63                     | 0.47              |
| 1:D:406:LYS:CD   | 1:D:406:LYS:H    | 2.11                     | 0.47              |
| 2:R:112:VAL:HB   | 1:X:443:ILE:HD12 | 1.96                     | 0.47              |
| 2:Q:133:ALA:O    | 2:Q:136:ALA:HB3  | 2.14                     | 0.47              |
| 1:E:352:LEU:O    | 1:E:355:GLN:N    | 2.48                     | 0.47              |
| 1:T:21:ALA:C     | 1:T:23:ALA:N     | 2.67                     | 0.47              |
| 2:P:153:LEU:HB3  | 2:P:167:PHE:CE2  | 2.50                     | 0.47              |
| 2:K:49:GLY:O     | 2:K:51:ALA:N     | 2.47                     | 0.47              |
| 2:I:105:ILE:O    | 2:I:105:ILE:HG23 | 2.15                     | 0.47              |
| 1:A:38:MET:HA    | 1:A:45:ARG:HH11  | 1.80                     | 0.47              |
| 1:U:96:VAL:HG21  | 1:U:281:ASP:HB3  | 1.96                     | 0.47              |
| 1:A:39:GLN:HG2   | 1:F:362:THR:HG21 | 1.93                     | 0.47              |
| 1:D:5:THR:O      | 1:D:9:ILE:HG13   | 2.15                     | 0.47              |
| 1:D:6:PRO:HD3    | 1:D:32:ARG:CG    | 2.45                     | 0.47              |
| 1:D:32:ARG:CZ    | 1:D:35:TRP:CE3   | 2.98                     | 0.47              |
| 1:C:37:ARG:NH1   | 1:C:38:MET:HE2   | 2.28                     | 0.47              |
| 1:V:21:ALA:C     | 1:V:23:ALA:N     | 2.65                     | 0.47              |
| 1:A:20:GLN:CA    | 1:A:20:GLN:HE21  | 2.28                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:283:LEU:HA   | 1:C:283:LEU:HD23 | 1.54                     | 0.47              |
| 1:T:61:VAL:HG11  | 1:T:335:ALA:HA   | 1.96                     | 0.47              |
| 1:V:254:VAL:HB   | 1:V:305:PHE:CD2  | 2.50                     | 0.47              |
| 1:B:236:ASN:N    | 1:B:237:PRO:HD3  | 2.30                     | 0.47              |
| 2:O:4:VAL:HG12   | 2:O:153:LEU:HD21 | 1.97                     | 0.47              |
| 2:R:49:GLY:O     | 2:R:51:ALA:N     | 2.48                     | 0.47              |
| 2:H:60:PHE:CE2   | 2:H:97:VAL:HG11  | 2.49                     | 0.47              |
| 1:S:28:ALA:C     | 1:S:30:ALA:H     | 2.17                     | 0.47              |
| 1:B:73:LEU:HD12  | 1:B:73:LEU:C     | 2.35                     | 0.47              |
| 2:J:7:ARG:CZ     | 2:J:12:VAL:HG22  | 2.44                     | 0.47              |
| 2:O:32:ARG:HB2   | 2:O:35:ARG:HE    | 1.80                     | 0.47              |
| 1:C:280:ARG:HG3  | 1:C:280:ARG:HH11 | 1.79                     | 0.47              |
| 1:T:17:ILE:HD13  | 1:T:66:ILE:HG13  | 1.96                     | 0.47              |
| 1:B:443:ILE:HG23 | 2:H:112:VAL:HG23 | 1.96                     | 0.47              |
| 1:V:100:ILE:HG13 | 1:V:291:VAL:HG21 | 1.95                     | 0.47              |
| 1:V:297:MET:CE   | 1:W:105:ASP:HB3  | 2.44                     | 0.47              |
| 2:K:133:ALA:HB1  | 2:K:155:ILE:HD12 | 1.97                     | 0.47              |
| 1:W:273:VAL:HG12 | 1:W:273:VAL:O    | 2.15                     | 0.47              |
| 1:U:17:ILE:O     | 1:U:17:ILE:HG22  | 2.14                     | 0.47              |
| 1:A:403:LEU:C    | 1:A:405:ASP:H    | 2.18                     | 0.47              |
| 2:J:2:THR:O      | 2:J:16:GLY:HA2   | 2.15                     | 0.47              |
| 2:N:1:THR:HG23   | 2:N:33:LYS:HD3   | 1.95                     | 0.47              |
| 1:F:250:GLN:NE2  | 1:F:250:GLN:CA   | 2.73                     | 0.47              |
| 1:B:338:ALA:N    | 1:B:382:PHE:CD1  | 2.80                     | 0.47              |
| 2:L:1:THR:HG22   | 2:L:2:THR:H      | 1.78                     | 0.47              |
| 2:I:137:LEU:HD13 | 2:O:136:ALA:HB1  | 1.95                     | 0.47              |
| 2:J:137:LEU:N    | 2:J:137:LEU:CD1  | 2.77                     | 0.47              |
| 2:J:140:ASN:C    | 2:J:141:THR:HG22 | 2.36                     | 0.47              |
| 1:C:275:ARG:O    | 1:C:277:GLY:N    | 2.48                     | 0.47              |
| 1:V:341:PHE:CB   | 1:V:378:ALA:HB1  | 2.45                     | 0.47              |
| 2:K:88:LEU:O     | 2:K:89:ARG:HB2   | 2.13                     | 0.47              |
| 1:S:48:VAL:HG23  | 1:T:355:GLN:OE1  | 2.15                     | 0.47              |
| 2:G:3:ILE:O      | 2:G:122:ALA:HA   | 2.15                     | 0.47              |
| 1:D:85:LYS:O     | 1:D:85:LYS:HG2   | 2.14                     | 0.47              |
| 1:T:357:LYS:CA   | 1:T:367:ILE:HD11 | 2.34                     | 0.47              |
| 1:S:427:ALA:C    | 1:S:429:ALA:H    | 2.18                     | 0.47              |
| 1:E:38:MET:HG3   | 1:E:45:ARG:HH12  | 1.79                     | 0.47              |
| 1:T:112:ARG:O    | 1:T:112:ARG:HG2  | 2.14                     | 0.47              |
| 1:C:37:ARG:HA    | 1:C:40:LEU:HD12  | 1.95                     | 0.47              |
| 1:U:61:VAL:HA    | 1:U:336:LEU:HD21 | 1.96                     | 0.47              |
| 2:M:144:SER:OG   | 2:M:147:GLU:HB2  | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:381:ALA:HB2  | 1:D:396:LEU:HD23 | 1.96                     | 0.47              |
| 2:P:107:THR:OG1  | 2:P:111:ASP:OD2  | 2.23                     | 0.47              |
| 2:L:3:ILE:O      | 2:L:122:ALA:HA   | 2.15                     | 0.47              |
| 1:S:279:GLN:O    | 1:S:320:ILE:HD11 | 2.15                     | 0.46              |
| 1:D:401:GLU:OE1  | 1:E:51:LYS:HG3   | 2.16                     | 0.46              |
| 2:Q:55:THR:HG22  | 2:R:83:ARG:CG    | 2.44                     | 0.46              |
| 2:I:78:LEU:HG    | 2:I:82:TRP:HZ3   | 1.80                     | 0.46              |
| 1:B:244:ALA:O    | 1:B:247:ALA:HB3  | 2.15                     | 0.46              |
| 1:F:38:MET:HA    | 1:F:45:ARG:HH11  | 1.79                     | 0.46              |
| 2:P:8:ARG:HH22   | 2:P:143:LEU:H    | 1.63                     | 0.46              |
| 2:H:7:ARG:NH2    | 2:H:102:GLU:O    | 2.48                     | 0.46              |
| 1:A:37:ARG:HB2   | 1:A:48:VAL:HG11  | 1.96                     | 0.46              |
| 1:S:9:ILE:HD13   | 1:S:31:LEU:HD23  | 1.97                     | 0.46              |
| 2:G:82:TRP:CE2   | 2:G:88:LEU:HD22  | 2.50                     | 0.46              |
| 1:C:236:ASN:O    | 1:C:240:LEU:HD13 | 2.15                     | 0.46              |
| 1:S:68:ARG:HG3   | 1:S:68:ARG:NH1   | 2.30                     | 0.46              |
| 2:H:71:LEU:C     | 2:H:71:LEU:HD13  | 2.35                     | 0.46              |
| 1:X:435:GLU:HB3  | 1:X:436:ASN:H    | 1.51                     | 0.46              |
| 1:S:45:ARG:O     | 1:S:48:VAL:HG12  | 2.15                     | 0.46              |
| 2:G:161:VAL:HG22 | 2:R:24:ASN:O     | 2.15                     | 0.46              |
| 1:D:110:LEU:O    | 1:D:114:GLN:HB2  | 2.15                     | 0.46              |
| 2:P:71:LEU:O     | 2:P:73:LYS:N     | 2.48                     | 0.46              |
| 1:F:115:GLU:OE2  | 1:F:118:LYS:HD3  | 2.15                     | 0.46              |
| 1:B:403:LEU:C    | 1:B:405:ASP:H    | 2.19                     | 0.46              |
| 1:B:311:PHE:CE1  | 1:B:316:PRO:HA   | 2.51                     | 0.46              |
| 1:E:240:LEU:O    | 1:E:243:LYS:N    | 2.48                     | 0.46              |
| 1:C:17:ILE:HA    | 3:C:452:ATP:C2   | 2.50                     | 0.46              |
| 2:Q:90:LYS:O     | 2:Q:91:LEU:HD12  | 2.15                     | 0.46              |
| 2:N:4:VAL:HG12   | 2:N:153:LEU:CD2  | 2.45                     | 0.46              |
| 1:B:367:ILE:HD11 | 1:B:421:ILE:HD11 | 1.96                     | 0.46              |
| 1:V:54:LEU:CD2   | 1:V:307:ALA:HB3  | 2.45                     | 0.46              |
| 1:V:48:VAL:CG2   | 1:W:359:LEU:HD11 | 2.44                     | 0.46              |
| 1:A:250:GLN:HA   | 1:A:250:GLN:HE21 | 1.80                     | 0.46              |
| 1:F:32:ARG:CZ    | 1:F:35:TRP:CE3   | 2.98                     | 0.46              |
| 1:W:48:VAL:HG21  | 1:X:359:LEU:HD11 | 1.96                     | 0.46              |
| 1:F:435:GLU:O    | 1:F:436:ASN:CB   | 2.62                     | 0.46              |
| 1:C:41:GLN:HE21  | 1:C:41:GLN:HA    | 1.79                     | 0.46              |
| 1:W:101:ARG:HA   | 1:W:293:THR:HG22 | 1.96                     | 0.46              |
| 1:W:28:ALA:C     | 1:W:30:ALA:N     | 2.68                     | 0.46              |
| 1:B:81:VAL:HG11  | 1:B:99:ILE:HG12  | 1.97                     | 0.46              |
| 2:I:133:ALA:HB1  | 2:I:155:ILE:HD12 | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:394:ARG:HA   | 1:E:394:ARG:HD3  | 1.78                     | 0.46              |
| 2:J:91:LEU:O     | 2:J:108:GLY:HA3  | 2.15                     | 0.46              |
| 1:U:260:ASP:HB3  | 1:U:311:PHE:HD2  | 1.77                     | 0.46              |
| 1:F:370:THR:O    | 1:F:373:ALA:N    | 2.45                     | 0.46              |
| 1:X:439:LEU:C    | 1:X:441:ARG:N    | 2.67                     | 0.46              |
| 1:A:439:LEU:HD23 | 2:G:72:LEU:HD11  | 1.98                     | 0.46              |
| 1:T:427:ALA:C    | 1:T:429:ALA:H    | 2.19                     | 0.46              |
| 1:B:108:MET:CE   | 1:B:240:LEU:HD23 | 2.45                     | 0.46              |
| 2:R:164:ASN:N    | 2:R:164:ASN:ND2  | 2.60                     | 0.46              |
| 1:S:350:ALA:HB2  | 1:X:47:GLU:OE1   | 2.16                     | 0.46              |
| 1:T:9:ILE:HD13   | 1:T:31:LEU:HD23  | 1.97                     | 0.46              |
| 1:X:9:ILE:O      | 1:X:13:LEU:HG    | 2.15                     | 0.46              |
| 1:E:366:ASN:O    | 1:E:418:THR:HA   | 2.15                     | 0.46              |
| 1:U:120:ARG:CG   | 1:U:232:ALA:HA   | 2.45                     | 0.46              |
| 2:J:70:HIS:O     | 2:J:71:LEU:C     | 2.53                     | 0.46              |
| 2:J:60:PHE:CE2   | 2:J:97:VAL:HG11  | 2.50                     | 0.46              |
| 1:W:68:ARG:HG3   | 1:W:68:ARG:NH1   | 2.31                     | 0.46              |
| 1:D:55:MET:CE    | 1:D:306:ILE:HG21 | 2.45                     | 0.46              |
| 1:U:430:LEU:HD23 | 1:U:430:LEU:N    | 2.31                     | 0.46              |
| 2:L:3:ILE:HG22   | 2:L:96:ILE:HD12  | 1.96                     | 0.46              |
| 2:K:98:ALA:HB2   | 2:K:103:SER:HA   | 1.98                     | 0.46              |
| 1:B:414:MET:O    | 1:B:414:MET:HG2  | 2.14                     | 0.46              |
| 2:R:151:LYS:O    | 2:R:155:ILE:HD13 | 2.15                     | 0.46              |
| 1:B:65:GLU:HG3   | 3:B:451:ATP:H2'  | 1.97                     | 0.46              |
| 1:A:403:LEU:CD1  | 1:A:426:VAL:HG22 | 2.46                     | 0.46              |
| 2:G:99:ASP:HA    | 2:G:172:LEU:CD1  | 2.46                     | 0.46              |
| 2:G:57:PHE:CA    | 2:G:95:LEU:HD11  | 2.41                     | 0.46              |
| 1:B:9:ILE:HD13   | 1:B:31:LEU:HD23  | 1.98                     | 0.46              |
| 2:N:8:ARG:HH22   | 2:N:143:LEU:H    | 1.63                     | 0.46              |
| 2:H:137:LEU:N    | 2:H:137:LEU:CD1  | 2.78                     | 0.46              |
| 2:Q:8:ARG:HH22   | 2:Q:143:LEU:H    | 1.63                     | 0.46              |
| 2:G:144:SER:CB   | 2:G:147:GLU:HG3  | 2.42                     | 0.46              |
| 1:X:17:ILE:O     | 1:X:17:ILE:HG22  | 2.15                     | 0.46              |
| 1:D:63:LYS:HB2   | 3:D:453:ATP:O2B  | 2.15                     | 0.46              |
| 2:O:7:ARG:NH1    | 2:O:12:VAL:HG21  | 2.30                     | 0.46              |
| 1:F:76:ALA:HB1   | 1:F:251:ASN:O    | 2.14                     | 0.46              |
| 1:S:336:LEU:HB2  | 1:S:341:PHE:CE1  | 2.51                     | 0.46              |
| 2:M:33:LYS:HA    | 2:M:46:PHE:CZ    | 2.51                     | 0.46              |
| 1:F:262:ILE:HG13 | 1:F:262:ILE:O    | 2.15                     | 0.46              |
| 1:C:116:ILE:O    | 1:C:120:ARG:HB2  | 2.16                     | 0.46              |
| 1:T:28:ALA:C     | 1:T:30:ALA:H     | 2.18                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:280:ARG:HD3  | 1:F:82:GLU:OE2   | 2.16                     | 0.46              |
| 1:A:360:MET:CA   | 1:A:360:MET:CE   | 2.94                     | 0.46              |
| 2:J:164:ASN:HD22 | 2:J:164:ASN:C    | 2.18                     | 0.46              |
| 1:A:234:LEU:O    | 1:A:235:ILE:C    | 2.54                     | 0.46              |
| 2:N:37:LEU:HD22  | 2:N:61:GLU:HG3   | 1.96                     | 0.46              |
| 1:U:442:PHE:N    | 1:U:442:PHE:CD1  | 2.83                     | 0.46              |
| 1:E:338:ALA:N    | 1:E:382:PHE:HD1  | 2.13                     | 0.46              |
| 1:E:37:ARG:NH1   | 1:E:38:MET:HE2   | 2.30                     | 0.46              |
| 1:V:385:ASN:ND2  | 1:V:395:ARG:HE   | 2.10                     | 0.46              |
| 2:J:38:TYR:CD1   | 2:J:69:GLY:HA3   | 2.50                     | 0.46              |
| 2:K:7:ARG:CZ     | 2:K:12:VAL:HG22  | 2.45                     | 0.46              |
| 2:H:159:ILE:O    | 2:M:25:THR:HA    | 2.16                     | 0.46              |
| 2:O:151:LYS:O    | 2:O:155:ILE:HD13 | 2.16                     | 0.46              |
| 2:N:35:ARG:HH11  | 2:N:35:ARG:HG3   | 1.80                     | 0.46              |
| 1:V:28:ALA:O     | 1:V:30:ALA:N     | 2.49                     | 0.46              |
| 2:R:7:ARG:NH1    | 2:R:12:VAL:HG21  | 2.30                     | 0.46              |
| 2:Q:56:LEU:CD2   | 2:Q:95:LEU:HD13  | 2.46                     | 0.46              |
| 2:L:55:THR:O     | 2:L:59:LEU:HD13  | 2.16                     | 0.46              |
| 2:H:52:ASP:OD2   | 2:H:91:LEU:HA    | 2.16                     | 0.46              |
| 1:U:427:ALA:C    | 1:U:429:ALA:H    | 2.19                     | 0.46              |
| 2:R:4:VAL:HA     | 2:R:121:LEU:O    | 2.16                     | 0.46              |
| 2:G:107:THR:OG1  | 2:G:109:ILE:HG12 | 2.16                     | 0.46              |
| 1:C:356:TYR:CE1  | 1:C:400:MET:HB3  | 2.48                     | 0.46              |
| 1:D:280:ARG:NH1  | 1:D:280:ARG:HG3  | 2.30                     | 0.46              |
| 1:X:351:SER:O    | 1:X:355:GLN:HG3  | 2.16                     | 0.46              |
| 1:D:384:VAL:HG22 | 1:D:385:ASN:N    | 2.31                     | 0.46              |
| 1:A:428:ASP:O    | 1:A:430:LEU:N    | 2.49                     | 0.46              |
| 1:T:28:ALA:O     | 1:T:30:ALA:N     | 2.49                     | 0.46              |
| 2:M:127:GLY:O    | 2:M:129:TYR:N    | 2.48                     | 0.46              |
| 2:H:85:ASP:O     | 2:H:87:ALA:N     | 2.49                     | 0.46              |
| 2:R:104:LEU:HD13 | 2:R:112:VAL:CG1  | 2.46                     | 0.46              |
| 2:N:56:LEU:HD23  | 2:N:95:LEU:HD13  | 1.98                     | 0.46              |
| 2:N:164:ASN:ND2  | 2:N:164:ASN:N    | 2.62                     | 0.46              |
| 2:I:2:THR:O      | 2:I:16:GLY:HA2   | 2.15                     | 0.46              |
| 3:D:453:ATP:H5'1 | 3:D:453:ATP:C8   | 2.51                     | 0.46              |
| 1:B:360:MET:CE   | 1:B:360:MET:CA   | 2.94                     | 0.46              |
| 1:U:120:ARG:HG3  | 1:U:232:ALA:CA   | 2.46                     | 0.46              |
| 1:S:61:VAL:HG11  | 1:S:335:ALA:HA   | 1.96                     | 0.46              |
| 1:F:112:ARG:HB2  | 1:F:240:LEU:HD21 | 1.96                     | 0.46              |
| 1:A:54:LEU:HG    | 1:A:56:ILE:HD11  | 1.98                     | 0.46              |
| 1:W:430:LEU:HD23 | 1:W:430:LEU:H    | 1.81                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:112:ARG:C    | 1:D:114:GLN:H    | 2.19                     | 0.46              |
| 1:V:28:ALA:C     | 1:V:30:ALA:H     | 2.18                     | 0.46              |
| 1:C:249:GLU:HG2  | 1:C:299:LYS:H    | 1.80                     | 0.46              |
| 1:A:74:ALA:O     | 1:A:75:ASN:C     | 2.53                     | 0.46              |
| 2:M:151:LYS:O    | 2:M:155:ILE:HD13 | 2.16                     | 0.46              |
| 1:B:428:ASP:O    | 1:B:430:LEU:N    | 2.49                     | 0.46              |
| 1:S:240:LEU:HD12 | 1:S:240:LEU:N    | 2.30                     | 0.46              |
| 1:X:322:GLU:N    | 1:X:322:GLU:OE1  | 2.48                     | 0.46              |
| 1:W:17:ILE:O     | 1:W:17:ILE:HG22  | 2.14                     | 0.46              |
| 1:T:283:LEU:CD1  | 1:T:323:LEU:HD12 | 2.45                     | 0.46              |
| 2:N:56:LEU:HB2   | 2:N:91:LEU:CD2   | 2.36                     | 0.46              |
| 1:E:369:PHE:CE2  | 1:E:421:ILE:HD12 | 2.51                     | 0.46              |
| 1:B:409:PHE:O    | 1:C:6:PRO:HG2    | 2.16                     | 0.46              |
| 2:M:4:VAL:HA     | 2:M:121:LEU:O    | 2.16                     | 0.46              |
| 2:M:42:VAL:HG21  | 2:M:64:LEU:CD1   | 2.46                     | 0.46              |
| 1:E:382:PHE:HD2  | 1:E:382:PHE:C    | 2.19                     | 0.46              |
| 1:A:41:GLN:NE2   | 1:A:41:GLN:CA    | 2.74                     | 0.46              |
| 1:A:25:ARG:O     | 1:A:28:ALA:HB3   | 2.15                     | 0.46              |
| 1:W:47:GLU:OE1   | 1:X:350:ALA:HB2  | 2.16                     | 0.46              |
| 1:S:430:LEU:HD23 | 1:S:430:LEU:H    | 1.79                     | 0.46              |
| 1:V:28:ALA:C     | 1:V:30:ALA:N     | 2.69                     | 0.46              |
| 1:T:265:LYS:H    | 1:T:269:SER:HB3  | 1.81                     | 0.46              |
| 1:S:119:ASN:O    | 1:S:234:LEU:HD22 | 2.16                     | 0.46              |
| 1:T:439:LEU:O    | 1:T:440:SER:C    | 2.53                     | 0.46              |
| 1:F:421:ILE:HG23 | 1:F:425:TYR:HD1  | 1.80                     | 0.46              |
| 2:M:90:LYS:C     | 2:M:91:LEU:HD12  | 2.36                     | 0.46              |
| 2:M:90:LYS:O     | 2:M:91:LEU:HD12  | 2.16                     | 0.46              |
| 2:H:83:ARG:HG2   | 2:I:55:THR:HB    | 1.97                     | 0.46              |
| 1:E:408:SER:O    | 1:F:36:ARG:NH2   | 2.37                     | 0.46              |
| 1:E:439:LEU:HA   | 1:E:443:ILE:CD1  | 2.46                     | 0.46              |
| 1:X:427:ALA:C    | 1:X:429:ALA:H    | 2.19                     | 0.46              |
| 2:G:54:PHE:O     | 2:G:55:THR:C     | 2.54                     | 0.46              |
| 1:X:65:GLU:HA    | 1:X:65:GLU:OE1   | 2.16                     | 0.46              |
| 2:O:131:LEU:HD12 | 2:O:135:ARG:HG3  | 1.98                     | 0.46              |
| 2:P:55:THR:O     | 2:P:59:LEU:HB2   | 2.16                     | 0.46              |
| 2:K:70:HIS:O     | 2:K:71:LEU:C     | 2.54                     | 0.46              |
| 1:B:76:ALA:HB1   | 1:B:251:ASN:O    | 2.16                     | 0.46              |
| 1:W:34:ARG:HG2   | 1:W:250:GLN:NE2  | 2.31                     | 0.46              |
| 1:V:101:ARG:HA   | 1:V:293:THR:HG22 | 1.97                     | 0.46              |
| 1:T:28:ALA:C     | 1:T:30:ALA:N     | 2.69                     | 0.46              |
| 1:A:381:ALA:HB2  | 1:A:396:LEU:HD23 | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:430:LEU:HD23 | 1:V:430:LEU:H    | 1.80                     | 0.46              |
| 1:F:378:ALA:O    | 1:F:379:GLU:C    | 2.52                     | 0.46              |
| 1:D:404:MET:O    | 1:D:408:SER:HB2  | 2.16                     | 0.46              |
| 1:X:369:PHE:HE2  | 1:X:421:ILE:CD1  | 2.21                     | 0.46              |
| 2:M:133:ALA:O    | 2:M:136:ALA:HB3  | 2.16                     | 0.46              |
| 2:K:86:ARG:CG    | 2:K:87:ALA:N     | 2.77                     | 0.46              |
| 1:X:18:ILE:CG2   | 1:X:344:ILE:HG13 | 2.46                     | 0.46              |
| 1:V:427:ALA:C    | 1:V:429:ALA:H    | 2.18                     | 0.46              |
| 1:C:33:ASN:HA    | 1:C:36:ARG:HD2   | 1.98                     | 0.46              |
| 1:E:341:PHE:O    | 1:E:345:LEU:HB2  | 2.16                     | 0.46              |
| 1:B:37:ARG:HG3   | 1:B:38:MET:N     | 2.31                     | 0.46              |
| 2:L:13:VAL:HG12  | 2:L:14:VAL:N     | 2.30                     | 0.46              |
| 1:U:51:LYS:HE2   | 1:V:356:TYR:OH   | 2.15                     | 0.46              |
| 1:V:119:ASN:HD22 | 1:V:119:ASN:C    | 2.18                     | 0.46              |
| 1:S:28:ALA:C     | 1:S:30:ALA:N     | 2.68                     | 0.46              |
| 1:A:9:ILE:O      | 1:A:10:VAL:C     | 2.54                     | 0.46              |
| 1:A:313:VAL:HG23 | 1:A:314:ALA:H    | 1.80                     | 0.46              |
| 2:G:115:PRO:HG3  | 2:G:121:LEU:HD11 | 1.98                     | 0.46              |
| 2:L:61:GLU:O     | 2:L:62:ARG:C     | 2.54                     | 0.46              |
| 1:U:273:VAL:O    | 1:U:273:VAL:HG12 | 2.15                     | 0.46              |
| 1:W:265:LYS:H    | 1:W:269:SER:HB3  | 1.79                     | 0.46              |
| 1:W:439:LEU:O    | 1:W:441:ARG:N    | 2.49                     | 0.45              |
| 1:W:441:ARG:O    | 1:W:443:ILE:N    | 2.49                     | 0.45              |
| 2:N:7:ARG:NH1    | 2:N:12:VAL:HG21  | 2.32                     | 0.45              |
| 1:F:403:LEU:HD23 | 1:F:404:MET:CA   | 2.45                     | 0.45              |
| 1:W:17:ILE:CD1   | 1:W:65:GLU:HB3   | 2.46                     | 0.45              |
| 1:B:58:PRO:HD2   | 1:B:61:VAL:HG21  | 1.97                     | 0.45              |
| 2:K:79:ALA:HB1   | 2:K:83:ARG:NH2   | 2.24                     | 0.45              |
| 2:M:153:LEU:HB3  | 2:M:167:PHE:CE2  | 2.51                     | 0.45              |
| 2:P:134:ALA:O    | 2:P:137:LEU:N    | 2.49                     | 0.45              |
| 1:X:17:ILE:HD13  | 1:X:66:ILE:HG13  | 1.97                     | 0.45              |
| 1:C:421:ILE:HG12 | 1:C:425:TYR:CE1  | 2.51                     | 0.45              |
| 1:B:347:GLU:N    | 1:B:348:PRO:CD   | 2.79                     | 0.45              |
| 1:W:61:VAL:HG11  | 1:W:335:ALA:HA   | 1.97                     | 0.45              |
| 1:D:51:LYS:O     | 1:D:52:ASN:O     | 2.33                     | 0.45              |
| 1:A:343:ARG:O    | 1:A:348:PRO:HD3  | 2.16                     | 0.45              |
| 1:X:351:SER:OG   | 1:X:354:GLU:HG2  | 2.16                     | 0.45              |
| 2:I:86:ARG:O     | 2:I:87:ALA:CB    | 2.64                     | 0.45              |
| 1:F:239:GLU:O    | 1:F:240:LEU:C    | 2.54                     | 0.45              |
| 1:S:430:LEU:HD23 | 1:S:430:LEU:N    | 2.31                     | 0.45              |
| 1:E:249:GLU:OE1  | 1:E:299:LYS:HG3  | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:33:LYS:HA    | 2:Q:46:PHE:CZ    | 2.51                     | 0.45              |
| 1:D:53:ILE:HG22  | 1:D:54:LEU:N     | 2.30                     | 0.45              |
| 2:N:94:MET:HE3   | 2:N:123:ILE:HB   | 1.99                     | 0.45              |
| 1:C:71:ALA:HB1   | 1:C:78:PHE:HB2   | 1.98                     | 0.45              |
| 1:F:44:LEU:HA    | 1:F:47:GLU:HB2   | 1.98                     | 0.45              |
| 1:W:322:GLU:HA   | 1:X:394:ARG:NH1  | 2.31                     | 0.45              |
| 2:N:113:VAL:HG22 | 1:T:444:LEU:HD21 | 1.99                     | 0.45              |
| 1:E:360:MET:CA   | 1:E:360:MET:CE   | 2.94                     | 0.45              |
| 1:E:357:LYS:HG2  | 1:E:367:ILE:HG23 | 1.99                     | 0.45              |
| 1:F:39:GLN:HE21  | 1:F:39:GLN:HB2   | 1.50                     | 0.45              |
| 1:T:17:ILE:HG22  | 1:T:17:ILE:O     | 2.15                     | 0.45              |
| 1:B:5:THR:O      | 1:B:6:PRO:C      | 2.54                     | 0.45              |
| 2:K:1:THR:CG2    | 2:K:33:LYS:NZ    | 2.79                     | 0.45              |
| 2:Q:42:VAL:HG21  | 2:Q:64:LEU:CD1   | 2.46                     | 0.45              |
| 1:B:283:LEU:HD23 | 1:B:283:LEU:HA   | 1.60                     | 0.45              |
| 1:E:300:THR:HA   | 1:E:303:ILE:HG12 | 1.97                     | 0.45              |
| 1:X:68:ARG:HG3   | 1:X:68:ARG:NH1   | 2.32                     | 0.45              |
| 1:X:101:ARG:HA   | 1:X:293:THR:HG22 | 1.97                     | 0.45              |
| 2:O:144:SER:OG   | 2:O:147:GLU:HB2  | 2.15                     | 0.45              |
| 1:T:273:VAL:O    | 1:T:273:VAL:HG12 | 2.16                     | 0.45              |
| 1:U:344:ILE:CG2  | 3:U:458:ATP:C2   | 2.99                     | 0.45              |
| 1:X:357:LYS:HA   | 1:X:367:ILE:CD1  | 2.32                     | 0.45              |
| 2:G:17:ASP:C     | 2:G:33:LYS:HD2   | 2.36                     | 0.45              |
| 1:B:5:THR:HG23   | 1:B:8:GLU:CD     | 2.36                     | 0.45              |
| 2:P:164:ASN:N    | 2:P:164:ASN:HD22 | 1.97                     | 0.45              |
| 1:B:38:MET:HG3   | 1:B:45:ARG:HH12  | 1.82                     | 0.45              |
| 2:Q:43:LEU:HD11  | 2:Q:172:LEU:HG   | 1.98                     | 0.45              |
| 1:C:34:ARG:NH2   | 1:C:253:ILE:HD13 | 2.30                     | 0.45              |
| 1:X:430:LEU:N    | 1:X:430:LEU:HD23 | 2.31                     | 0.45              |
| 2:K:155:ILE:O    | 2:K:159:ILE:HG13 | 2.16                     | 0.45              |
| 2:P:32:ARG:HB2   | 2:P:35:ARG:HE    | 1.81                     | 0.45              |
| 1:B:249:GLU:HG2  | 1:B:299:LYS:H    | 1.81                     | 0.45              |
| 1:S:18:ILE:HD11  | 1:S:343:ARG:HH21 | 1.81                     | 0.45              |
| 2:I:1:THR:CG2    | 2:I:33:LYS:HD3   | 2.46                     | 0.45              |
| 1:X:63:LYS:H     | 3:X:461:ATP:PB   | 2.40                     | 0.45              |
| 1:D:108:MET:CE   | 1:D:241:LYS:HA   | 2.46                     | 0.45              |
| 1:B:321:PRO:HA   | 1:B:324:GLN:HB3  | 1.97                     | 0.45              |
| 1:D:283:LEU:CB   | 1:D:284:PRO:HD3  | 2.43                     | 0.45              |
| 1:V:430:LEU:HG   | 1:V:431:GLY:H    | 1.81                     | 0.45              |
| 1:X:28:ALA:C     | 1:X:30:ALA:H     | 2.20                     | 0.45              |
| 1:T:433:VAL:HG12 | 1:T:434:VAL:N    | 2.32                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:25:ARG:O     | 1:C:28:ALA:HB3   | 2.16                     | 0.45              |
| 1:B:233:LYS:O    | 1:B:233:LYS:HG2  | 2.17                     | 0.45              |
| 2:R:42:VAL:HG21  | 2:R:64:LEU:CD1   | 2.47                     | 0.45              |
| 2:N:90:LYS:C     | 2:N:91:LEU:HD12  | 2.36                     | 0.45              |
| 1:W:427:ALA:C    | 1:W:429:ALA:H    | 2.20                     | 0.45              |
| 1:B:108:MET:O    | 1:B:109:LYS:C    | 2.54                     | 0.45              |
| 2:J:136:ALA:HB1  | 2:P:137:LEU:HD13 | 1.99                     | 0.45              |
| 1:D:410:SER:O    | 1:D:411:ALA:C    | 2.53                     | 0.45              |
| 2:G:13:VAL:CG2   | 2:G:171:GLU:HB3  | 2.45                     | 0.45              |
| 1:X:361:ALA:C    | 1:X:363:GLU:H    | 2.19                     | 0.45              |
| 1:C:357:LYS:HE3  | 1:C:367:ILE:O    | 2.17                     | 0.45              |
| 1:B:444:LEU:HD21 | 2:I:20:VAL:HG21  | 1.98                     | 0.45              |
| 1:V:65:GLU:HA    | 1:V:65:GLU:OE1   | 2.17                     | 0.45              |
| 1:F:356:TYR:O    | 1:F:357:LYS:C    | 2.55                     | 0.45              |
| 1:T:254:VAL:HB   | 1:T:305:PHE:CD2  | 2.52                     | 0.45              |
| 1:S:39:GLN:HB2   | 1:T:362:THR:HG21 | 1.99                     | 0.45              |
| 1:B:384:VAL:O    | 1:B:385:ASN:C    | 2.55                     | 0.45              |
| 1:A:31:LEU:HD21  | 1:A:74:ALA:HB2   | 1.98                     | 0.45              |
| 1:F:347:GLU:N    | 1:F:348:PRO:CD   | 2.79                     | 0.45              |
| 1:D:25:ARG:O     | 1:D:28:ALA:HB3   | 2.16                     | 0.45              |
| 2:K:73:LYS:O     | 2:K:74:SER:C     | 2.54                     | 0.45              |
| 2:H:172:LEU:HA   | 2:H:172:LEU:HD23 | 1.75                     | 0.45              |
| 2:Q:7:ARG:NH1    | 2:Q:12:VAL:HG21  | 2.31                     | 0.45              |
| 1:S:283:LEU:CD1  | 1:S:323:LEU:HD12 | 2.46                     | 0.45              |
| 1:B:403:LEU:CD2  | 1:B:404:MET:N    | 2.74                     | 0.45              |
| 1:X:357:LYS:CA   | 1:X:367:ILE:HD11 | 2.33                     | 0.45              |
| 1:E:356:TYR:O    | 1:E:357:LYS:C    | 2.55                     | 0.45              |
| 1:F:441:ARG:NH1  | 2:G:36:ARG:O     | 2.50                     | 0.45              |
| 2:L:1:THR:CG2    | 2:L:2:THR:N      | 2.79                     | 0.45              |
| 1:X:18:ILE:HD11  | 1:X:343:ARG:HH21 | 1.81                     | 0.45              |
| 1:X:227:ILE:N    | 1:X:230:GLU:HB2  | 2.32                     | 0.45              |
| 1:X:96:VAL:HG21  | 1:X:281:ASP:HB3  | 1.98                     | 0.45              |
| 1:B:283:LEU:CB   | 1:B:284:PRO:CD   | 2.95                     | 0.45              |
| 1:E:4:MET:CE     | 1:E:9:ILE:HA     | 2.47                     | 0.45              |
| 1:F:34:ARG:NH2   | 1:F:253:ILE:HD13 | 2.32                     | 0.45              |
| 1:W:387:LYS:NZ   | 1:W:435:GLU:HG3  | 2.31                     | 0.45              |
| 1:F:339:ALA:O    | 1:F:342:GLU:HB2  | 2.17                     | 0.45              |
| 1:X:265:LYS:H    | 1:X:269:SER:HB3  | 1.79                     | 0.45              |
| 2:G:165:THR:HA   | 2:G:167:PHE:CE2  | 2.51                     | 0.45              |
| 1:U:265:LYS:H    | 1:U:269:SER:HB3  | 1.81                     | 0.45              |
| 1:X:279:GLN:O    | 1:X:320:ILE:HD11 | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:62:GLY:O     | 1:A:63:LYS:C     | 2.54                     | 0.45              |
| 1:S:344:ILE:HG22 | 1:S:344:ILE:O    | 2.16                     | 0.45              |
| 1:D:38:MET:HA    | 1:D:45:ARG:HH11  | 1.82                     | 0.45              |
| 1:F:443:ILE:CD1  | 2:L:72:LEU:HD11  | 2.44                     | 0.45              |
| 2:K:42:VAL:HG21  | 2:K:64:LEU:HD13  | 1.99                     | 0.45              |
| 1:A:326:ARG:C    | 1:A:328:PRO:HD3  | 2.37                     | 0.45              |
| 1:U:61:VAL:HG11  | 1:U:335:ALA:HA   | 1.98                     | 0.45              |
| 1:A:283:LEU:HD23 | 1:A:283:LEU:HA   | 1.79                     | 0.45              |
| 2:L:86:ARG:HB3   | 2:L:87:ALA:H     | 1.48                     | 0.45              |
| 1:C:108:MET:O    | 1:C:110:LEU:N    | 2.50                     | 0.45              |
| 1:C:249:GLU:OE1  | 1:C:299:LYS:HG3  | 2.17                     | 0.45              |
| 2:M:92:GLU:O     | 2:M:93:ALA:HB2   | 2.16                     | 0.45              |
| 2:M:157:GLY:HA2  | 2:M:163:THR:HG22 | 1.99                     | 0.45              |
| 1:U:28:ALA:C     | 1:U:30:ALA:H     | 2.20                     | 0.45              |
| 1:X:273:VAL:HG12 | 1:X:273:VAL:O    | 2.16                     | 0.45              |
| 1:C:360:MET:CE   | 1:C:360:MET:HA   | 2.47                     | 0.45              |
| 1:F:421:ILE:HA   | 1:F:425:TYR:HD1  | 1.81                     | 0.45              |
| 1:F:428:ASP:O    | 1:F:430:LEU:N    | 2.50                     | 0.45              |
| 1:U:18:ILE:HG22  | 1:U:344:ILE:HG12 | 1.99                     | 0.45              |
| 1:C:60:GLY:HA2   | 3:C:452:ATP:PB   | 2.56                     | 0.45              |
| 1:T:331:VAL:O    | 1:T:331:VAL:HG13 | 2.17                     | 0.45              |
| 1:E:439:LEU:HA   | 1:E:443:ILE:HG13 | 1.97                     | 0.45              |
| 1:S:17:ILE:CD1   | 1:S:65:GLU:HB3   | 2.46                     | 0.45              |
| 1:B:377:ILE:HD13 | 1:B:400:MET:SD   | 2.57                     | 0.45              |
| 1:S:260:ASP:HB3  | 1:S:311:PHE:HD2  | 1.74                     | 0.45              |
| 1:D:17:ILE:HG22  | 1:D:18:ILE:N     | 2.31                     | 0.45              |
| 1:D:5:THR:O      | 1:D:6:PRO:C      | 2.56                     | 0.45              |
| 1:C:250:GLN:HE21 | 1:C:250:GLN:CA   | 2.27                     | 0.45              |
| 2:P:35:ARG:HH11  | 2:P:35:ARG:HG3   | 1.80                     | 0.45              |
| 1:C:374:VAL:O    | 1:C:375:LYS:C    | 2.55                     | 0.45              |
| 1:W:119:ASN:ND2  | 1:W:119:ASN:O    | 2.50                     | 0.45              |
| 2:J:36:ARG:NH1   | 2:J:170:GLU:OE2  | 2.50                     | 0.45              |
| 1:B:64:THR:N     | 3:B:451:ATP:O2B  | 2.42                     | 0.45              |
| 1:U:357:LYS:CA   | 1:U:367:ILE:HD11 | 2.32                     | 0.45              |
| 2:P:90:LYS:O     | 2:P:91:LEU:HD12  | 2.17                     | 0.45              |
| 2:G:137:LEU:HD13 | 2:M:136:ALA:HB1  | 1.93                     | 0.45              |
| 1:C:338:ALA:N    | 1:C:382:PHE:CD1  | 2.85                     | 0.45              |
| 2:H:164:ASN:N    | 2:H:164:ASN:HD22 | 2.13                     | 0.45              |
| 2:H:7:ARG:CZ     | 2:H:12:VAL:HG22  | 2.45                     | 0.45              |
| 1:W:36:ARG:HH11  | 1:X:363:GLU:HG2  | 1.82                     | 0.45              |
| 1:S:101:ARG:HA   | 1:S:293:THR:HG22 | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:236:ASN:O    | 1:S:239:GLU:HB3  | 2.17                     | 0.45              |
| 1:D:381:ALA:CB   | 1:D:396:LEU:HD23 | 2.47                     | 0.45              |
| 1:W:329:ILE:HG12 | 1:X:401:GLU:HG2  | 1.99                     | 0.45              |
| 2:K:115:PRO:HG3  | 2:K:121:LEU:HD11 | 1.99                     | 0.45              |
| 2:Q:92:GLU:O     | 2:Q:93:ALA:HB2   | 2.17                     | 0.45              |
| 2:G:164:ASN:C    | 2:G:164:ASN:ND2  | 2.70                     | 0.45              |
| 1:A:233:LYS:HZ3  | 1:A:234:LEU:HB2  | 1.82                     | 0.45              |
| 1:C:107:ALA:CB   | 1:C:248:VAL:HG23 | 2.47                     | 0.45              |
| 1:D:33:ASN:HA    | 1:D:36:ARG:HD2   | 1.98                     | 0.45              |
| 1:A:108:MET:HG3  | 1:A:295:HIS:CE1  | 2.51                     | 0.45              |
| 1:B:438:ASP:CG   | 1:B:439:LEU:H    | 2.19                     | 0.45              |
| 1:V:20:GLN:O     | 1:V:21:ALA:CB    | 2.65                     | 0.45              |
| 1:D:360:MET:CA   | 1:D:360:MET:CE   | 2.94                     | 0.45              |
| 1:W:344:ILE:O    | 1:W:344:ILE:HG22 | 2.17                     | 0.45              |
| 2:Q:107:THR:OG1  | 2:Q:111:ASP:OD2  | 2.24                     | 0.45              |
| 2:M:82:TRP:CE3   | 2:M:110:GLY:HA2  | 2.52                     | 0.45              |
| 1:X:75:ASN:HD22  | 1:X:75:ASN:HA    | 1.53                     | 0.45              |
| 1:F:340:ASP:O    | 1:F:344:ILE:CD1  | 2.65                     | 0.44              |
| 1:W:55:MET:HE2   | 1:W:306:ILE:CG2  | 2.46                     | 0.44              |
| 1:A:403:LEU:HD11 | 1:A:426:VAL:HG22 | 2.00                     | 0.44              |
| 1:B:227:ILE:CG1  | 1:B:227:ILE:O    | 2.64                     | 0.44              |
| 2:I:52:ASP:OD2   | 2:I:91:LEU:HA    | 2.17                     | 0.44              |
| 2:L:141:THR:HG21 | 2:L:143:LEU:HD12 | 1.99                     | 0.44              |
| 2:Q:5:SER:N      | 2:Q:121:LEU:O    | 2.45                     | 0.44              |
| 1:A:382:PHE:O    | 1:A:383:ARG:C    | 2.55                     | 0.44              |
| 1:E:37:ARG:HG2   | 1:E:38:MET:N     | 2.32                     | 0.44              |
| 1:X:235:ILE:HG22 | 1:X:236:ASN:N    | 2.32                     | 0.44              |
| 1:A:79:ILE:CG2   | 1:A:103:LEU:HD13 | 2.44                     | 0.44              |
| 1:C:283:LEU:CB   | 1:C:284:PRO:HD3  | 2.45                     | 0.44              |
| 1:A:34:ARG:NH2   | 1:A:253:ILE:HD13 | 2.32                     | 0.44              |
| 1:V:430:LEU:HD23 | 1:V:430:LEU:N    | 2.32                     | 0.44              |
| 1:W:118:LYS:HG2  | 1:W:119:ASN:N    | 2.32                     | 0.44              |
| 2:R:2:THR:O      | 2:R:16:GLY:HA2   | 2.17                     | 0.44              |
| 1:W:109:LYS:O    | 1:W:113:GLN:HB2  | 2.17                     | 0.44              |
| 2:L:60:PHE:CE2   | 2:L:97:VAL:HG11  | 2.52                     | 0.44              |
| 2:R:71:LEU:O     | 2:R:73:LYS:N     | 2.50                     | 0.44              |
| 2:M:104:LEU:HD13 | 2:M:112:VAL:CG1  | 2.48                     | 0.44              |
| 1:V:283:LEU:CD1  | 1:V:323:LEU:HD12 | 2.48                     | 0.44              |
| 1:B:264:LYS:NZ   | 1:B:319:LEU:HA   | 2.32                     | 0.44              |
| 1:B:231:ALA:CA   | 1:B:234:LEU:HD21 | 2.34                     | 0.44              |
| 1:E:403:LEU:CD2  | 1:E:404:MET:HG2  | 2.45                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:65:GLU:OE1   | 1:S:65:GLU:HA    | 2.17                     | 0.44              |
| 2:G:77:GLU:HA    | 2:G:80:LYS:HG2   | 1.97                     | 0.44              |
| 1:D:76:ALA:HB1   | 1:D:251:ASN:O    | 2.17                     | 0.44              |
| 2:K:17:ASP:HB2   | 2:K:164:ASN:HD21 | 1.81                     | 0.44              |
| 1:X:344:ILE:O    | 1:X:344:ILE:HG22 | 2.17                     | 0.44              |
| 1:E:280:ARG:HA   | 1:E:283:LEU:HD12 | 1.99                     | 0.44              |
| 2:J:117:GLU:C    | 2:J:119:GLN:H    | 2.21                     | 0.44              |
| 1:W:36:ARG:CA    | 1:W:36:ARG:HE    | 2.29                     | 0.44              |
| 1:D:116:ILE:CG1  | 1:D:117:ALA:N    | 2.80                     | 0.44              |
| 1:C:100:ILE:HG22 | 1:C:298:VAL:HG21 | 1.97                     | 0.44              |
| 1:V:55:MET:HE3   | 1:V:255:PHE:HE1  | 1.83                     | 0.44              |
| 1:W:336:LEU:HB2  | 1:W:341:PHE:HE1  | 1.81                     | 0.44              |
| 1:F:41:GLN:O     | 1:F:43:PRO:HD2   | 2.17                     | 0.44              |
| 2:J:71:LEU:C     | 2:J:71:LEU:HD13  | 2.38                     | 0.44              |
| 1:T:344:ILE:HG22 | 1:T:344:ILE:O    | 2.16                     | 0.44              |
| 2:P:82:TRP:CE3   | 2:P:110:GLY:HA2  | 2.52                     | 0.44              |
| 1:A:12:GLU:O     | 1:A:15:GLN:HB2   | 2.17                     | 0.44              |
| 2:M:35:ARG:HG3   | 2:M:35:ARG:HH11  | 1.81                     | 0.44              |
| 2:H:36:ARG:NH1   | 2:H:170:GLU:OE2  | 2.50                     | 0.44              |
| 2:K:2:THR:O      | 2:K:16:GLY:HA2   | 2.17                     | 0.44              |
| 1:W:283:LEU:CD1  | 1:W:323:LEU:HD12 | 2.46                     | 0.44              |
| 1:E:52:ASN:HB2   | 1:E:326:ARG:O    | 2.17                     | 0.44              |
| 2:I:82:TRP:CE2   | 2:I:108:GLY:O    | 2.70                     | 0.44              |
| 1:T:368:ALA:HB3  | 1:T:420:ASN:HA   | 1.99                     | 0.44              |
| 1:S:17:ILE:O     | 1:S:17:ILE:HG22  | 2.16                     | 0.44              |
| 2:M:8:ARG:HH22   | 2:M:143:LEU:H    | 1.66                     | 0.44              |
| 1:U:435:GLU:CG   | 1:U:436:ASN:N    | 2.80                     | 0.44              |
| 1:X:55:MET:HE2   | 1:X:306:ILE:HG21 | 1.99                     | 0.44              |
| 1:D:37:ARG:HH12  | 1:D:38:MET:HE2   | 1.82                     | 0.44              |
| 2:R:52:ASP:HA    | 2:R:55:THR:OG1   | 2.17                     | 0.44              |
| 1:U:336:LEU:HB2  | 1:U:341:PHE:CE1  | 2.52                     | 0.44              |
| 1:V:341:PHE:HB2  | 1:V:378:ALA:HB1  | 1.99                     | 0.44              |
| 1:T:101:ARG:HA   | 1:T:293:THR:HG22 | 1.98                     | 0.44              |
| 1:F:410:SER:O    | 1:F:411:ALA:C    | 2.56                     | 0.44              |
| 2:O:107:THR:OG1  | 2:O:111:ASP:OD2  | 2.25                     | 0.44              |
| 1:B:29:ILE:HG13  | 1:B:30:ALA:N     | 2.32                     | 0.44              |
| 1:F:71:ALA:HB1   | 1:F:78:PHE:HB2   | 2.00                     | 0.44              |
| 1:V:112:ARG:O    | 1:V:112:ARG:HG2  | 2.17                     | 0.44              |
| 1:A:394:ARG:HA   | 1:A:394:ARG:HD3  | 1.74                     | 0.44              |
| 1:T:436:ASN:O    | 1:T:437:GLU:C    | 2.56                     | 0.44              |
| 1:W:279:GLN:HE22 | 1:W:319:LEU:CA   | 2.30                     | 0.44              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:82:TRP:CE3   | 2:I:110:GLY:HA2  | 2.52                     | 0.44              |
| 2:I:89:ARG:O     | 2:I:90:LYS:CB    | 2.65                     | 0.44              |
| 2:N:164:ASN:HD22 | 2:N:164:ASN:N    | 2.01                     | 0.44              |
| 2:R:33:LYS:HA    | 2:R:46:PHE:CZ    | 2.52                     | 0.44              |
| 2:I:1:THR:CG2    | 2:I:33:LYS:NZ    | 2.81                     | 0.44              |
| 1:F:60:GLY:CA    | 3:F:455:ATP:O1B  | 2.65                     | 0.44              |
| 1:V:369:PHE:HE2  | 1:V:421:ILE:CD1  | 2.24                     | 0.44              |
| 1:E:382:PHE:O    | 1:E:383:ARG:C    | 2.56                     | 0.44              |
| 1:D:407:ILE:O    | 1:D:411:ALA:CB   | 2.63                     | 0.44              |
| 2:P:7:ARG:NH1    | 2:P:12:VAL:HG21  | 2.32                     | 0.44              |
| 1:C:421:ILE:HG12 | 1:C:425:TYR:CD1  | 2.51                     | 0.44              |
| 1:U:233:LYS:HA   | 1:U:235:ILE:HG12 | 2.00                     | 0.44              |
| 1:S:36:ARG:NE    | 1:S:36:ARG:HA    | 2.31                     | 0.44              |
| 1:F:56:ILE:N     | 1:F:56:ILE:CD1   | 2.79                     | 0.44              |
| 1:X:61:VAL:HG12  | 1:X:336:LEU:HG   | 1.99                     | 0.44              |
| 1:V:345:LEU:HD21 | 1:V:377:ILE:HG22 | 1.99                     | 0.44              |
| 2:R:144:SER:OG   | 2:R:147:GLU:HB2  | 2.17                     | 0.44              |
| 2:M:43:LEU:HD11  | 2:M:172:LEU:HG   | 1.99                     | 0.44              |
| 2:O:157:GLY:HA2  | 2:O:163:THR:HG22 | 1.99                     | 0.44              |
| 1:E:81:VAL:HG11  | 1:E:99:ILE:HG12  | 2.00                     | 0.44              |
| 1:U:351:SER:OG   | 1:U:354:GLU:HG2  | 2.18                     | 0.44              |
| 2:R:75:ALA:O     | 2:R:78:LEU:HB3   | 2.17                     | 0.44              |
| 2:P:13:VAL:HG13  | 2:P:171:GLU:HB3  | 2.00                     | 0.44              |
| 2:L:172:LEU:HA   | 2:L:172:LEU:HD23 | 1.64                     | 0.44              |
| 2:Q:7:ARG:NH2    | 2:Q:102:GLU:O    | 2.50                     | 0.44              |
| 2:I:83:ARG:HG2   | 2:J:55:THR:HB    | 1.97                     | 0.44              |
| 1:E:51:LYS:O     | 1:E:52:ASN:O     | 2.35                     | 0.44              |
| 1:E:352:LEU:O    | 1:E:355:GLN:HB2  | 2.17                     | 0.44              |
| 2:G:17:ASP:HB2   | 2:G:164:ASN:HD21 | 1.75                     | 0.44              |
| 1:T:54:LEU:CD2   | 1:T:307:ALA:HB3  | 2.47                     | 0.44              |
| 1:S:20:GLN:O     | 1:S:21:ALA:CB    | 2.66                     | 0.44              |
| 2:H:91:LEU:O     | 2:H:108:GLY:HA3  | 2.18                     | 0.44              |
| 2:K:1:THR:HG23   | 2:K:33:LYS:CD    | 2.46                     | 0.44              |
| 1:D:442:PHE:CD2  | 2:J:76:VAL:HG11  | 2.52                     | 0.44              |
| 1:B:79:ILE:HD12  | 1:B:80:LYS:H     | 1.83                     | 0.44              |
| 1:E:414:MET:O    | 1:E:417:GLN:HG3  | 2.17                     | 0.44              |
| 1:W:385:ASN:ND2  | 1:W:395:ARG:HE   | 2.14                     | 0.44              |
| 1:E:313:VAL:HG23 | 1:E:314:ALA:N    | 2.31                     | 0.44              |
| 1:V:436:ASN:O    | 1:V:437:GLU:C    | 2.56                     | 0.44              |
| 2:I:155:ILE:O    | 2:I:159:ILE:HG13 | 2.18                     | 0.44              |
| 1:A:381:ALA:O    | 1:A:384:VAL:HG13 | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:321:PRO:HA   | 1:A:324:GLN:HB3  | 2.00                     | 0.44              |
| 2:J:67:HIS:CD2   | 2:J:73:LYS:HD3   | 2.52                     | 0.44              |
| 1:D:264:LYS:CE   | 1:D:279:GLN:HE22 | 2.27                     | 0.44              |
| 1:B:227:ILE:O    | 1:B:230:GLU:HB3  | 2.17                     | 0.44              |
| 1:S:344:ILE:O    | 1:S:344:ILE:CG2  | 2.65                     | 0.44              |
| 1:B:20:GLN:HG3   | 1:B:333:LEU:HD23 | 1.99                     | 0.44              |
| 1:F:13:LEU:CD1   | 1:F:24:LYS:HG2   | 2.47                     | 0.44              |
| 1:W:32:ARG:NH2   | 1:X:363:GLU:OE1  | 2.48                     | 0.44              |
| 1:C:404:MET:O    | 1:C:408:SER:HB2  | 2.17                     | 0.44              |
| 2:I:136:ALA:HB1  | 2:O:137:LEU:HD13 | 1.99                     | 0.44              |
| 1:S:36:ARG:HE    | 1:S:36:ARG:CA    | 2.29                     | 0.44              |
| 1:F:283:LEU:O    | 1:F:285:LEU:N    | 2.51                     | 0.44              |
| 1:V:68:ARG:HG3   | 1:V:68:ARG:NH1   | 2.32                     | 0.44              |
| 1:T:68:ARG:HG3   | 1:T:68:ARG:NH1   | 2.32                     | 0.44              |
| 1:T:18:ILE:HD11  | 1:T:343:ARG:NH2  | 2.32                     | 0.44              |
| 1:T:351:SER:OG   | 1:T:354:GLU:HG2  | 2.17                     | 0.44              |
| 1:X:265:LYS:H    | 1:X:269:SER:CB   | 2.31                     | 0.44              |
| 2:N:144:SER:OG   | 2:N:147:GLU:HB2  | 2.17                     | 0.44              |
| 1:U:361:ALA:C    | 1:U:363:GLU:H    | 2.20                     | 0.44              |
| 1:B:322:GLU:OE2  | 1:B:322:GLU:N    | 2.44                     | 0.44              |
| 1:F:378:ALA:C    | 1:F:380:ALA:N    | 2.71                     | 0.44              |
| 1:X:442:PHE:O    | 1:X:443:ILE:HD13 | 2.18                     | 0.44              |
| 1:T:235:ILE:CG2  | 1:T:236:ASN:N    | 2.80                     | 0.44              |
| 1:B:4:MET:HE3    | 1:B:8:GLU:HG2    | 1.98                     | 0.44              |
| 2:I:17:ASP:CG    | 2:I:163:THR:HG23 | 2.38                     | 0.44              |
| 1:T:300:THR:O    | 1:T:302:HIS:N    | 2.50                     | 0.44              |
| 1:E:338:ALA:O    | 1:E:341:PHE:HB2  | 2.17                     | 0.44              |
| 1:F:360:MET:CA   | 1:F:360:MET:CE   | 2.96                     | 0.44              |
| 1:F:360:MET:N    | 1:F:360:MET:HE2  | 2.33                     | 0.44              |
| 1:A:293:THR:C    | 1:A:295:HIS:H    | 2.21                     | 0.44              |
| 1:B:262:ILE:HG13 | 1:B:262:ILE:O    | 2.18                     | 0.44              |
| 1:V:36:ARG:CA    | 1:V:36:ARG:HE    | 2.30                     | 0.44              |
| 1:U:36:ARG:CA    | 1:U:36:ARG:HE    | 2.30                     | 0.44              |
| 1:T:430:LEU:HD23 | 1:T:430:LEU:H    | 1.81                     | 0.44              |
| 1:T:430:LEU:HD23 | 1:T:430:LEU:N    | 2.33                     | 0.44              |
| 1:V:361:ALA:C    | 1:V:363:GLU:H    | 2.21                     | 0.44              |
| 1:A:300:THR:HA   | 1:A:303:ILE:HG12 | 1.99                     | 0.44              |
| 2:O:92:GLU:O     | 2:O:93:ALA:HB2   | 2.18                     | 0.44              |
| 1:U:53:ILE:HG12  | 1:U:329:ILE:HB   | 1.99                     | 0.44              |
| 1:X:368:ALA:HB3  | 1:X:420:ASN:HA   | 1.99                     | 0.44              |
| 1:A:361:ALA:O    | 1:A:364:GLY:N    | 2.41                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:49:GLY:O     | 2:G:50:THR:C     | 2.55                     | 0.44              |
| 2:R:116:GLU:O    | 2:R:117:GLU:C    | 2.56                     | 0.44              |
| 1:V:368:ALA:HB3  | 1:V:420:ASN:HA   | 2.00                     | 0.44              |
| 1:T:441:ARG:NH1  | 1:T:441:ARG:HG3  | 2.33                     | 0.44              |
| 1:F:425:TYR:O    | 1:F:428:ASP:HB3  | 2.18                     | 0.44              |
| 1:U:344:ILE:CG2  | 3:U:458:ATP:H2   | 2.29                     | 0.44              |
| 1:A:403:LEU:HD23 | 1:A:404:MET:CA   | 2.48                     | 0.44              |
| 1:T:17:ILE:CD1   | 1:T:65:GLU:HB3   | 2.45                     | 0.44              |
| 2:H:42:VAL:HG21  | 2:H:64:LEU:HD13  | 2.00                     | 0.44              |
| 1:B:293:THR:C    | 1:B:295:HIS:N    | 2.71                     | 0.44              |
| 1:S:55:MET:HE1   | 1:S:63:LYS:O     | 2.18                     | 0.44              |
| 2:H:141:THR:HG21 | 2:H:143:LEU:HD12 | 2.00                     | 0.44              |
| 3:F:455:ATP:H5'1 | 3:F:455:ATP:C8   | 2.53                     | 0.44              |
| 1:E:343:ARG:C    | 1:E:345:LEU:N    | 2.66                     | 0.44              |
| 1:D:357:LYS:HA   | 1:D:367:ILE:CG2  | 2.47                     | 0.44              |
| 1:D:3:GLU:CG     | 1:D:4:MET:N      | 2.81                     | 0.44              |
| 2:O:35:ARG:HG3   | 2:O:35:ARG:HH11  | 1.83                     | 0.44              |
| 2:N:32:ARG:HH11  | 2:N:32:ARG:HG3   | 1.83                     | 0.44              |
| 1:B:119:ASN:O    | 1:B:120:ARG:C    | 2.55                     | 0.44              |
| 2:N:127:GLY:O    | 2:N:129:TYR:N    | 2.51                     | 0.44              |
| 2:J:49:GLY:O     | 2:J:51:ALA:N     | 2.51                     | 0.44              |
| 2:M:107:THR:OG1  | 2:M:111:ASP:OD2  | 2.22                     | 0.44              |
| 1:U:55:MET:HE3   | 1:U:255:PHE:HE1  | 1.83                     | 0.44              |
| 1:T:55:MET:HE2   | 1:T:306:ILE:HG21 | 1.99                     | 0.44              |
| 1:T:65:GLU:HA    | 1:T:65:GLU:OE1   | 2.17                     | 0.44              |
| 1:A:58:PRO:O     | 1:A:63:LYS:NZ    | 2.37                     | 0.44              |
| 1:S:64:THR:OG1   | 1:S:255:PHE:HE2  | 2.01                     | 0.44              |
| 2:I:164:ASN:C    | 2:I:164:ASN:ND2  | 2.71                     | 0.44              |
| 1:D:108:MET:HG3  | 1:D:295:HIS:CE1  | 2.52                     | 0.44              |
| 1:B:360:MET:CE   | 1:C:36:ARG:NH1   | 2.80                     | 0.44              |
| 1:C:100:ILE:HG13 | 1:C:300:THR:CG2  | 2.48                     | 0.44              |
| 1:B:436:ASN:HB3  | 1:B:439:LEU:HD11 | 2.00                     | 0.44              |
| 1:E:100:ILE:CG2  | 1:E:298:VAL:HG21 | 2.48                     | 0.44              |
| 1:V:344:ILE:O    | 1:V:344:ILE:HG22 | 2.17                     | 0.44              |
| 1:A:53:ILE:CG2   | 1:A:54:LEU:N     | 2.81                     | 0.44              |
| 1:C:315:ARG:O    | 1:C:318:ASP:HB2  | 2.18                     | 0.44              |
| 2:I:154:ARG:O    | 2:I:155:ILE:C    | 2.55                     | 0.44              |
| 2:M:32:ARG:HB2   | 2:M:35:ARG:HE    | 1.83                     | 0.44              |
| 2:I:25:THR:HA    | 2:N:159:ILE:O    | 2.17                     | 0.44              |
| 1:S:111:VAL:O    | 1:S:115:GLU:HB2  | 2.18                     | 0.44              |
| 1:V:265:LYS:H    | 1:V:269:SER:HB3  | 1.82                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:437:GLU:O    | 1:S:438:ASP:C    | 2.57                     | 0.43              |
| 1:U:65:GLU:CG    | 3:U:458:ATP:H5'2 | 2.30                     | 0.43              |
| 1:E:111:VAL:O    | 1:E:111:VAL:HG12 | 2.18                     | 0.43              |
| 1:B:357:LYS:HE3  | 1:B:367:ILE:O    | 2.17                     | 0.43              |
| 2:R:5:SER:N      | 2:R:121:LEU:O    | 2.45                     | 0.43              |
| 1:C:23:ALA:CA    | 1:C:331:VAL:HG21 | 2.43                     | 0.43              |
| 1:A:337:SER:O    | 1:A:340:ASP:HB2  | 2.17                     | 0.43              |
| 1:U:439:LEU:C    | 1:U:441:ARG:H    | 2.21                     | 0.43              |
| 2:L:105:ILE:O    | 2:L:105:ILE:HG23 | 2.17                     | 0.43              |
| 2:K:13:VAL:HG12  | 2:K:14:VAL:N     | 2.32                     | 0.43              |
| 2:M:49:GLY:O     | 2:M:51:ALA:N     | 2.51                     | 0.43              |
| 1:D:374:VAL:O    | 1:D:375:LYS:C    | 2.57                     | 0.43              |
| 2:Q:157:GLY:HA2  | 2:Q:163:THR:HG22 | 1.99                     | 0.43              |
| 1:V:279:GLN:O    | 1:V:320:ILE:HD11 | 2.17                     | 0.43              |
| 1:F:382:PHE:CD2  | 1:F:382:PHE:C    | 2.91                     | 0.43              |
| 1:F:428:ASP:OD1  | 1:F:429:ALA:N    | 2.51                     | 0.43              |
| 1:U:66:ILE:O     | 1:U:66:ILE:HG22  | 2.18                     | 0.43              |
| 2:K:83:ARG:CG    | 2:L:55:THR:HG22  | 2.38                     | 0.43              |
| 1:B:293:THR:O    | 1:B:295:HIS:N    | 2.51                     | 0.43              |
| 1:X:353:THR:HG22 | 1:X:369:PHE:HD1  | 1.82                     | 0.43              |
| 1:F:107:ALA:CB   | 1:F:248:VAL:HG23 | 2.48                     | 0.43              |
| 1:D:60:GLY:HA2   | 3:D:453:ATP:O1B  | 2.18                     | 0.43              |
| 1:F:79:ILE:HD12  | 1:F:80:LYS:H     | 1.83                     | 0.43              |
| 1:V:9:ILE:O      | 1:V:13:LEU:HG    | 2.19                     | 0.43              |
| 2:O:55:THR:HG22  | 2:P:83:ARG:HA    | 2.00                     | 0.43              |
| 1:V:34:ARG:HG2   | 1:V:250:GLN:NE2  | 2.32                     | 0.43              |
| 1:D:29:ILE:HG13  | 1:D:30:ALA:N     | 2.33                     | 0.43              |
| 1:W:361:ALA:C    | 1:W:363:GLU:H    | 2.22                     | 0.43              |
| 2:Q:82:TRP:CE3   | 2:Q:110:GLY:HA2  | 2.53                     | 0.43              |
| 1:X:111:VAL:HG11 | 1:X:244:ALA:HA   | 2.00                     | 0.43              |
| 1:W:351:SER:OG   | 1:W:354:GLU:HG2  | 2.18                     | 0.43              |
| 1:D:336:LEU:HD12 | 1:D:336:LEU:HA   | 1.65                     | 0.43              |
| 1:W:439:LEU:HD23 | 1:W:439:LEU:N    | 2.33                     | 0.43              |
| 1:T:441:ARG:O    | 1:T:443:ILE:N    | 2.50                     | 0.43              |
| 1:X:279:GLN:HE22 | 1:X:319:LEU:CA   | 2.31                     | 0.43              |
| 2:M:56:LEU:HD23  | 2:M:95:LEU:HD13  | 1.99                     | 0.43              |
| 2:N:113:VAL:HG22 | 1:T:444:LEU:CD2  | 2.48                     | 0.43              |
| 2:I:157:GLY:HA2  | 2:I:163:THR:HB   | 2.01                     | 0.43              |
| 1:V:54:LEU:HD21  | 1:V:327:LEU:CD1  | 2.41                     | 0.43              |
| 1:F:16:HIS:C     | 1:F:17:ILE:HD12  | 2.39                     | 0.43              |
| 1:E:283:LEU:O    | 1:E:287:GLU:HB2  | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:293:THR:C    | 1:D:295:HIS:H    | 2.20                     | 0.43              |
| 2:N:42:VAL:HG21  | 2:N:64:LEU:CD1   | 2.49                     | 0.43              |
| 1:C:107:ALA:HB2  | 1:C:248:VAL:CG2  | 2.48                     | 0.43              |
| 1:E:6:PRO:O      | 1:E:10:VAL:HG23  | 2.19                     | 0.43              |
| 1:A:39:GLN:HG2   | 1:F:362:THR:HG23 | 1.97                     | 0.43              |
| 1:A:114:GLN:HE21 | 1:A:114:GLN:HB3  | 1.57                     | 0.43              |
| 1:E:381:ALA:O    | 1:E:384:VAL:HG13 | 2.17                     | 0.43              |
| 1:C:260:ASP:HB3  | 1:C:311:PHE:CE2  | 2.52                     | 0.43              |
| 1:T:344:ILE:CG2  | 1:T:344:ILE:O    | 2.66                     | 0.43              |
| 1:W:430:LEU:N    | 1:W:430:LEU:HD23 | 2.33                     | 0.43              |
| 1:S:34:ARG:HG2   | 1:S:250:GLN:NE2  | 2.32                     | 0.43              |
| 1:E:347:GLU:N    | 1:E:348:PRO:CD   | 2.81                     | 0.43              |
| 2:G:3:ILE:HG22   | 2:G:96:ILE:HD12  | 2.00                     | 0.43              |
| 1:W:265:LYS:H    | 1:W:269:SER:CB   | 2.31                     | 0.43              |
| 2:M:13:VAL:HG13  | 2:M:171:GLU:HB3  | 2.00                     | 0.43              |
| 2:N:157:GLY:HA2  | 2:N:163:THR:HG22 | 2.00                     | 0.43              |
| 1:V:351:SER:OG   | 1:V:354:GLU:HG2  | 2.17                     | 0.43              |
| 1:F:264:LYS:HD3  | 1:F:276:GLU:CD   | 2.38                     | 0.43              |
| 1:D:264:LYS:O    | 1:D:265:LYS:HB3  | 2.18                     | 0.43              |
| 1:X:283:LEU:CD1  | 1:X:323:LEU:HD12 | 2.47                     | 0.43              |
| 1:D:403:LEU:CD2  | 1:D:404:MET:N    | 2.74                     | 0.43              |
| 1:D:101:ARG:HA   | 1:D:293:THR:HG22 | 2.00                     | 0.43              |
| 1:E:108:MET:HG3  | 1:E:295:HIS:NE2  | 2.33                     | 0.43              |
| 2:H:105:ILE:HD11 | 2:H:123:ILE:HG22 | 1.99                     | 0.43              |
| 2:O:112:VAL:HB   | 1:U:443:ILE:HD12 | 2.01                     | 0.43              |
| 1:D:409:PHE:CE1  | 1:E:6:PRO:HB3    | 2.53                     | 0.43              |
| 1:D:341:PHE:O    | 1:D:345:LEU:HB2  | 2.18                     | 0.43              |
| 1:W:18:ILE:HD11  | 1:W:343:ARG:NH2  | 2.33                     | 0.43              |
| 1:A:257:ASP:OD1  | 1:A:308:SER:OG   | 2.37                     | 0.43              |
| 2:N:82:TRP:CE3   | 2:N:110:GLY:HA2  | 2.53                     | 0.43              |
| 2:Q:35:ARG:HG3   | 2:Q:35:ARG:HH11  | 1.83                     | 0.43              |
| 1:W:20:GLN:O     | 1:W:21:ALA:CB    | 2.66                     | 0.43              |
| 1:U:55:MET:HE2   | 1:U:306:ILE:CG2  | 2.47                     | 0.43              |
| 2:Q:120:ILE:HD11 | 2:Q:138:VAL:HG21 | 2.01                     | 0.43              |
| 1:S:18:ILE:CG2   | 1:S:344:ILE:CG1  | 2.97                     | 0.43              |
| 2:H:52:ASP:HA    | 2:H:55:THR:CG2   | 2.43                     | 0.43              |
| 2:J:83:ARG:NH1   | 2:K:58:GLU:OE2   | 2.51                     | 0.43              |
| 1:B:357:LYS:NZ   | 1:B:368:ALA:HA   | 2.34                     | 0.43              |
| 2:L:107:THR:OG1  | 2:L:109:ILE:HG12 | 2.19                     | 0.43              |
| 1:F:439:LEU:CD2  | 2:L:72:LEU:HG    | 2.49                     | 0.43              |
| 1:F:100:ILE:HG22 | 1:F:298:VAL:HG21 | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:86:ARG:O     | 2:J:87:ALA:HB2   | 2.17                     | 0.43              |
| 1:F:55:MET:C     | 1:F:56:ILE:HD12  | 2.38                     | 0.43              |
| 1:V:336:LEU:HB2  | 1:V:341:PHE:CE1  | 2.53                     | 0.43              |
| 1:S:51:LYS:HE2   | 1:T:356:TYR:OH   | 2.18                     | 0.43              |
| 2:K:154:ARG:O    | 2:K:155:ILE:C    | 2.57                     | 0.43              |
| 1:U:110:LEU:O    | 1:U:114:GLN:HB2  | 2.18                     | 0.43              |
| 1:F:336:LEU:HD12 | 1:F:336:LEU:HA   | 1.74                     | 0.43              |
| 1:S:262:ILE:HD12 | 1:S:279:GLN:HB2  | 2.01                     | 0.43              |
| 1:S:322:GLU:OE1  | 1:S:322:GLU:N    | 2.51                     | 0.43              |
| 1:W:55:MET:HE3   | 1:W:255:PHE:HE1  | 1.82                     | 0.43              |
| 1:F:36:ARG:O     | 1:F:39:GLN:CB    | 2.63                     | 0.43              |
| 1:A:336:LEU:HA   | 1:A:336:LEU:HD12 | 1.70                     | 0.43              |
| 2:L:164:ASN:H    | 2:L:164:ASN:ND2  | 2.16                     | 0.43              |
| 1:E:57:GLY:HA3   | 1:E:63:LYS:HE3   | 2.00                     | 0.43              |
| 1:W:9:ILE:O      | 1:W:13:LEU:HG    | 2.18                     | 0.43              |
| 2:K:46:PHE:HB3   | 2:K:95:LEU:HD21  | 1.99                     | 0.43              |
| 2:N:134:ALA:O    | 2:N:137:LEU:N    | 2.51                     | 0.43              |
| 1:E:100:ILE:HG22 | 1:E:298:VAL:HG21 | 2.01                     | 0.43              |
| 1:U:36:ARG:NE    | 1:U:36:ARG:HA    | 2.31                     | 0.43              |
| 1:C:237:PRO:HB3  | 1:C:241:LYS:NZ   | 2.33                     | 0.43              |
| 1:D:360:MET:O    | 1:D:361:ALA:C    | 2.57                     | 0.43              |
| 2:N:154:ARG:O    | 2:N:155:ILE:C    | 2.57                     | 0.43              |
| 2:M:6:VAL:HG21   | 2:M:148:ILE:CG2  | 2.49                     | 0.43              |
| 2:L:49:GLY:O     | 2:L:50:THR:C     | 2.57                     | 0.43              |
| 1:C:428:ASP:O    | 1:C:430:LEU:N    | 2.51                     | 0.43              |
| 2:J:19:GLN:OE1   | 2:J:162:PHE:HA   | 2.18                     | 0.43              |
| 1:S:273:VAL:O    | 1:S:273:VAL:HG12 | 2.18                     | 0.43              |
| 1:C:336:LEU:HD12 | 1:C:336:LEU:HA   | 1.81                     | 0.43              |
| 2:K:85:ASP:N     | 2:K:85:ASP:OD1   | 2.51                     | 0.43              |
| 1:X:234:LEU:HD13 | 1:X:234:LEU:C    | 2.39                     | 0.43              |
| 1:W:63:LYS:N     | 3:W:460:ATP:O2B  | 2.52                     | 0.43              |
| 1:B:57:GLY:CA    | 1:B:63:LYS:HE3   | 2.48                     | 0.43              |
| 1:W:279:GLN:O    | 1:W:320:ILE:HD11 | 2.19                     | 0.43              |
| 1:E:239:GLU:O    | 1:E:243:LYS:HB2  | 2.19                     | 0.43              |
| 1:E:403:LEU:HD23 | 1:E:404:MET:CA   | 2.49                     | 0.43              |
| 1:E:19:GLY:O     | 1:E:20:GLN:C     | 2.55                     | 0.43              |
| 2:Q:120:ILE:HD13 | 2:Q:134:ALA:HB1  | 2.01                     | 0.43              |
| 2:L:42:VAL:HG21  | 2:L:64:LEU:HD13  | 1.99                     | 0.43              |
| 1:B:241:LYS:O    | 1:B:244:ALA:N    | 2.51                     | 0.43              |
| 1:F:20:GLN:OE1   | 1:F:333:LEU:HB3  | 2.17                     | 0.43              |
| 1:V:55:MET:HE2   | 1:V:306:ILE:HG21 | 2.01                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:410:SER:C    | 1:A:412:SER:N    | 2.72                     | 0.43              |
| 1:A:347:GLU:N    | 1:A:348:PRO:CD   | 2.82                     | 0.43              |
| 2:L:6:VAL:CG1    | 2:L:7:ARG:N      | 2.81                     | 0.43              |
| 2:O:49:GLY:O     | 2:O:51:ALA:N     | 2.52                     | 0.43              |
| 1:A:396:LEU:HA   | 1:A:396:LEU:HD23 | 1.80                     | 0.43              |
| 1:W:107:ALA:C    | 1:W:109:LYS:H    | 2.22                     | 0.43              |
| 2:K:36:ARG:NH1   | 2:K:170:GLU:OE2  | 2.52                     | 0.43              |
| 1:S:53:ILE:HG12  | 1:S:329:ILE:HB   | 2.00                     | 0.43              |
| 2:P:2:THR:O      | 2:P:16:GLY:HA2   | 2.18                     | 0.43              |
| 2:R:35:ARG:HG3   | 2:R:35:ARG:HH11  | 1.82                     | 0.43              |
| 2:J:91:LEU:CD1   | 2:J:91:LEU:N     | 2.64                     | 0.43              |
| 1:U:279:GLN:HE22 | 1:U:319:LEU:CA   | 2.31                     | 0.43              |
| 1:W:65:GLU:HA    | 1:W:65:GLU:OE1   | 2.18                     | 0.43              |
| 2:J:1:THR:CG2    | 2:J:33:LYS:NZ    | 2.82                     | 0.43              |
| 2:L:46:PHE:HB3   | 2:L:95:LEU:HD21  | 1.97                     | 0.43              |
| 1:A:439:LEU:O    | 1:A:440:SER:C    | 2.58                     | 0.43              |
| 1:W:353:THR:HG22 | 1:W:369:PHE:HD1  | 1.84                     | 0.43              |
| 1:W:259:ILE:HG23 | 1:W:260:ASP:N    | 2.34                     | 0.43              |
| 1:D:352:LEU:O    | 1:D:355:GLN:HB2  | 2.19                     | 0.43              |
| 1:E:344:ILE:HG22 | 3:E:454:ATP:C2   | 2.52                     | 0.43              |
| 2:K:46:PHE:HB3   | 2:K:95:LEU:HD23  | 2.01                     | 0.43              |
| 2:G:60:PHE:HA    | 2:G:78:LEU:HD22  | 2.00                     | 0.43              |
| 1:C:357:LYS:HA   | 1:C:367:ILE:CG2  | 2.48                     | 0.43              |
| 1:A:112:ARG:C    | 1:A:114:GLN:N    | 2.70                     | 0.43              |
| 1:D:283:LEU:HD23 | 1:D:283:LEU:HA   | 1.87                     | 0.43              |
| 1:S:79:ILE:O     | 1:S:79:ILE:HG23  | 2.19                     | 0.43              |
| 1:U:68:ARG:HG3   | 1:U:68:ARG:NH1   | 2.33                     | 0.43              |
| 1:X:28:ALA:O     | 1:X:30:ALA:N     | 2.51                     | 0.43              |
| 1:T:361:ALA:C    | 1:T:363:GLU:H    | 2.21                     | 0.43              |
| 2:O:2:THR:O      | 2:O:16:GLY:HA2   | 2.18                     | 0.43              |
| 1:E:363:GLU:HB3  | 1:E:411:ALA:O    | 2.18                     | 0.43              |
| 1:S:437:GLU:O    | 1:S:439:LEU:N    | 2.52                     | 0.43              |
| 1:T:279:GLN:HE22 | 1:T:319:LEU:CA   | 2.32                     | 0.43              |
| 1:U:65:GLU:OE1   | 1:U:65:GLU:HA    | 2.18                     | 0.43              |
| 1:D:403:LEU:C    | 1:D:405:ASP:H    | 2.20                     | 0.43              |
| 1:E:357:LYS:HA   | 1:E:367:ILE:CG2  | 2.48                     | 0.43              |
| 1:C:6:PRO:O      | 1:C:10:VAL:HG23  | 2.18                     | 0.43              |
| 1:U:300:THR:O    | 1:U:302:HIS:N    | 2.52                     | 0.43              |
| 1:F:433:VAL:CG1  | 1:F:434:VAL:H    | 2.23                     | 0.43              |
| 1:B:241:LYS:O    | 1:B:242:GLN:C    | 2.56                     | 0.43              |
| 2:R:17:ASP:OD2   | 2:R:33:LYS:HE3   | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:18:GLY:N     | 2:I:164:ASN:HD21 | 2.06                     | 0.43              |
| 1:X:331:VAL:HG13 | 1:X:331:VAL:O    | 2.19                     | 0.43              |
| 1:D:37:ARG:HB2   | 1:D:48:VAL:HG11  | 2.01                     | 0.43              |
| 1:D:58:PRO:HD2   | 1:D:61:VAL:HG21  | 1.99                     | 0.43              |
| 1:A:37:ARG:HG2   | 1:A:38:MET:N     | 2.34                     | 0.43              |
| 1:U:439:LEU:HA   | 1:U:443:ILE:HB   | 2.01                     | 0.43              |
| 1:C:37:ARG:HA    | 1:C:40:LEU:CD1   | 2.49                     | 0.43              |
| 1:X:356:TYR:CD1  | 1:X:404:MET:HG3  | 2.54                     | 0.43              |
| 2:K:60:PHE:HZ    | 2:K:71:LEU:HD22  | 1.83                     | 0.43              |
| 1:B:381:ALA:CB   | 1:B:396:LEU:HD23 | 2.48                     | 0.43              |
| 2:O:33:LYS:HA    | 2:O:46:PHE:CZ    | 2.54                     | 0.43              |
| 1:X:28:ALA:C     | 1:X:30:ALA:N     | 2.72                     | 0.43              |
| 2:R:13:VAL:HG21  | 2:R:146:HIS:HA   | 2.00                     | 0.43              |
| 2:I:61:GLU:O     | 2:I:62:ARG:C     | 2.55                     | 0.43              |
| 2:P:138:VAL:HG23 | 2:P:148:ILE:HD13 | 2.00                     | 0.43              |
| 1:T:329:ILE:HG12 | 1:U:401:GLU:HG2  | 2.00                     | 0.43              |
| 1:A:351:SER:O    | 1:A:355:GLN:HG3  | 2.18                     | 0.43              |
| 1:X:366:ASN:HD22 | 1:X:366:ASN:HA   | 1.63                     | 0.43              |
| 1:W:441:ARG:HD3  | 1:W:441:ARG:HA   | 1.78                     | 0.43              |
| 1:E:264:LYS:HZ1  | 1:E:319:LEU:HA   | 1.84                     | 0.43              |
| 1:W:283:LEU:N    | 1:W:284:PRO:CD   | 2.82                     | 0.43              |
| 2:R:83:ARG:NH1   | 1:X:442:PHE:HB2  | 2.34                     | 0.43              |
| 2:P:17:ASP:OD2   | 2:P:33:LYS:HE3   | 2.18                     | 0.43              |
| 2:K:86:ARG:O     | 2:L:89:ARG:HD3   | 2.18                     | 0.43              |
| 1:F:60:GLY:HA2   | 3:F:455:ATP:PB   | 2.59                     | 0.43              |
| 1:F:58:PRO:HD2   | 1:F:61:VAL:HG21  | 2.00                     | 0.43              |
| 1:X:344:ILE:O    | 1:X:344:ILE:CG2  | 2.66                     | 0.43              |
| 2:H:7:ARG:HA     | 2:H:11:GLN:O     | 2.19                     | 0.43              |
| 1:B:79:ILE:HD12  | 1:B:80:LYS:N     | 2.34                     | 0.43              |
| 1:S:361:ALA:C    | 1:S:363:GLU:H    | 2.22                     | 0.43              |
| 1:B:37:ARG:O     | 1:B:38:MET:HB3   | 2.19                     | 0.43              |
| 1:D:283:LEU:HD11 | 1:D:320:ILE:HD12 | 2.01                     | 0.43              |
| 2:H:115:PRO:HG3  | 2:H:121:LEU:HD21 | 2.01                     | 0.43              |
| 1:W:79:ILE:HG23  | 1:W:79:ILE:O     | 2.18                     | 0.43              |
| 2:G:61:GLU:O     | 2:G:64:LEU:N     | 2.52                     | 0.43              |
| 1:D:84:THR:C     | 1:D:86:PHE:N     | 2.69                     | 0.43              |
| 1:E:237:PRO:O    | 1:E:238:GLU:C    | 2.57                     | 0.43              |
| 1:A:390:ASN:HB2  | 2:G:68:GLN:OE1   | 2.18                     | 0.43              |
| 2:K:157:GLY:HA2  | 2:K:163:THR:HB   | 2.00                     | 0.43              |
| 1:E:264:LYS:CE   | 1:E:279:GLN:NE2  | 2.80                     | 0.42              |
| 1:S:439:LEU:C    | 1:S:441:ARG:H    | 2.21                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:401:GLU:OE1  | 1:C:51:LYS:HG3   | 2.19                     | 0.42              |
| 1:E:35:TRP:O     | 1:E:39:GLN:HB2   | 2.18                     | 0.42              |
| 1:W:319:LEU:O    | 1:W:324:GLN:NE2  | 2.52                     | 0.42              |
| 1:E:111:VAL:HG12 | 1:E:240:LEU:CD1  | 2.48                     | 0.42              |
| 2:Q:4:VAL:HG12   | 2:Q:153:LEU:HD21 | 2.01                     | 0.42              |
| 2:I:18:GLY:H     | 2:I:164:ASN:ND2  | 2.06                     | 0.42              |
| 1:A:250:GLN:HE21 | 1:A:250:GLN:CA   | 2.32                     | 0.42              |
| 1:D:443:ILE:HG22 | 1:D:444:LEU:N    | 2.34                     | 0.42              |
| 1:U:345:LEU:HD21 | 1:U:377:ILE:HG22 | 2.01                     | 0.42              |
| 2:O:134:ALA:O    | 2:O:137:LEU:N    | 2.52                     | 0.42              |
| 1:A:410:SER:O    | 1:A:411:ALA:C    | 2.53                     | 0.42              |
| 1:S:345:LEU:HD13 | 1:S:396:LEU:HD22 | 2.01                     | 0.42              |
| 1:W:344:ILE:O    | 1:W:344:ILE:CG2  | 2.67                     | 0.42              |
| 1:C:110:LEU:HA   | 1:C:110:LEU:HD12 | 1.86                     | 0.42              |
| 1:T:34:ARG:HG2   | 1:T:250:GLN:NE2  | 2.34                     | 0.42              |
| 1:U:34:ARG:HG2   | 1:U:250:GLN:NE2  | 2.34                     | 0.42              |
| 2:P:6:VAL:HG21   | 2:P:148:ILE:CG2  | 2.49                     | 0.42              |
| 1:U:324:GLN:HE22 | 1:V:389:GLU:HG2  | 1.84                     | 0.42              |
| 1:F:398:THR:HG22 | 1:F:399:VAL:N    | 2.32                     | 0.42              |
| 1:V:366:ASN:HA   | 1:V:366:ASN:HD22 | 1.65                     | 0.42              |
| 1:F:404:MET:O    | 1:F:408:SER:HB2  | 2.18                     | 0.42              |
| 1:T:283:LEU:CD1  | 1:T:322:GLU:HB3  | 2.50                     | 0.42              |
| 1:A:360:MET:HA   | 1:A:360:MET:HE1  | 2.01                     | 0.42              |
| 2:M:91:LEU:HB2   | 2:M:108:GLY:HA3  | 2.02                     | 0.42              |
| 2:Q:90:LYS:C     | 2:Q:91:LEU:HD12  | 2.39                     | 0.42              |
| 1:S:63:LYS:H     | 3:S:456:ATP:PB   | 2.42                     | 0.42              |
| 1:C:340:ASP:O    | 1:C:344:ILE:CD1  | 2.67                     | 0.42              |
| 2:L:18:GLY:N     | 2:L:164:ASN:HD21 | 2.06                     | 0.42              |
| 1:D:34:ARG:NH2   | 1:D:253:ILE:CD1  | 2.82                     | 0.42              |
| 1:F:18:ILE:N     | 3:F:455:ATP:N1   | 2.52                     | 0.42              |
| 1:V:421:ILE:HG12 | 1:V:425:TYR:CD1  | 2.54                     | 0.42              |
| 1:S:300:THR:O    | 1:S:302:HIS:N    | 2.51                     | 0.42              |
| 2:L:103:SER:O    | 2:L:104:LEU:CD1  | 2.64                     | 0.42              |
| 2:K:5:SER:CB     | 2:K:14:VAL:HG22  | 2.48                     | 0.42              |
| 1:C:283:LEU:HD11 | 1:C:320:ILE:CD1  | 2.49                     | 0.42              |
| 1:T:36:ARG:HE    | 1:T:36:ARG:CA    | 2.30                     | 0.42              |
| 1:A:410:SER:O    | 1:A:412:SER:N    | 2.52                     | 0.42              |
| 1:X:407:ILE:HG23 | 1:X:408:SER:N    | 2.34                     | 0.42              |
| 1:F:243:LYS:O    | 1:F:246:ASP:N    | 2.53                     | 0.42              |
| 2:N:32:ARG:HB2   | 2:N:35:ARG:HE    | 1.83                     | 0.42              |
| 2:M:32:ARG:HG3   | 2:M:32:ARG:HH11  | 1.83                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:265:LYS:H    | 1:S:269:SER:HB3  | 1.83                     | 0.42              |
| 1:S:368:ALA:HB3  | 1:S:420:ASN:HA   | 2.01                     | 0.42              |
| 2:Q:116:GLU:O    | 2:Q:117:GLU:C    | 2.57                     | 0.42              |
| 1:S:394:ARG:HH12 | 1:X:322:GLU:HG3  | 1.84                     | 0.42              |
| 2:I:17:ASP:HB2   | 2:I:164:ASN:HD21 | 1.76                     | 0.42              |
| 2:G:83:ARG:HH11  | 2:G:83:ARG:HG2   | 1.84                     | 0.42              |
| 2:H:75:ALA:O     | 2:H:78:LEU:HB3   | 2.19                     | 0.42              |
| 2:H:88:LEU:O     | 2:H:89:ARG:C     | 2.55                     | 0.42              |
| 2:R:4:VAL:HG12   | 2:R:153:LEU:CD2  | 2.49                     | 0.42              |
| 1:D:108:MET:CE   | 1:D:240:LEU:HG   | 2.49                     | 0.42              |
| 1:A:37:ARG:NH1   | 1:A:38:MET:HE2   | 2.33                     | 0.42              |
| 2:P:42:VAL:HG21  | 2:P:64:LEU:CD1   | 2.49                     | 0.42              |
| 1:C:359:LEU:HD12 | 1:D:36:ARG:HB3   | 2.02                     | 0.42              |
| 1:F:101:ARG:HA   | 1:F:293:THR:HG22 | 2.02                     | 0.42              |
| 1:D:326:ARG:C    | 1:D:328:PRO:HD3  | 2.39                     | 0.42              |
| 1:X:79:ILE:HG23  | 1:X:79:ILE:O     | 2.19                     | 0.42              |
| 1:X:34:ARG:HG2   | 1:X:250:GLN:NE2  | 2.34                     | 0.42              |
| 1:A:341:PHE:HA   | 1:A:344:ILE:CG1  | 2.49                     | 0.42              |
| 1:A:17:ILE:HB    | 1:A:24:LYS:HE3   | 2.01                     | 0.42              |
| 2:H:84:THR:HB    | 2:H:85:ASP:H     | 1.65                     | 0.42              |
| 1:W:53:ILE:HG12  | 1:W:329:ILE:HB   | 2.01                     | 0.42              |
| 1:S:283:LEU:N    | 1:S:284:PRO:CD   | 2.83                     | 0.42              |
| 1:U:344:ILE:HD13 | 3:U:458:ATP:N1   | 2.34                     | 0.42              |
| 2:Q:52:ASP:HA    | 2:Q:55:THR:OG1   | 2.19                     | 0.42              |
| 1:T:20:GLN:O     | 1:T:21:ALA:CB    | 2.67                     | 0.42              |
| 2:P:4:VAL:HA     | 2:P:121:LEU:O    | 2.18                     | 0.42              |
| 1:X:35:TRP:C     | 1:X:37:ARG:N     | 2.72                     | 0.42              |
| 1:A:367:ILE:HD11 | 1:A:421:ILE:HD12 | 2.00                     | 0.42              |
| 1:X:36:ARG:NE    | 1:X:36:ARG:HA    | 2.33                     | 0.42              |
| 1:C:4:MET:CE     | 1:C:9:ILE:HA     | 2.49                     | 0.42              |
| 2:P:43:LEU:O     | 2:P:97:VAL:HA    | 2.20                     | 0.42              |
| 1:A:20:GLN:NE2   | 1:A:20:GLN:HA    | 2.35                     | 0.42              |
| 1:W:341:PHE:CB   | 1:W:378:ALA:HB1  | 2.50                     | 0.42              |
| 1:T:79:ILE:HG23  | 1:T:79:ILE:O     | 2.20                     | 0.42              |
| 1:W:387:LYS:NZ   | 1:W:435:GLU:CG   | 2.83                     | 0.42              |
| 1:C:311:PHE:CE1  | 1:C:316:PRO:HA   | 2.53                     | 0.42              |
| 2:G:4:VAL:HG23   | 2:G:122:ALA:HB2  | 2.00                     | 0.42              |
| 1:E:410:SER:O    | 1:E:412:SER:N    | 2.53                     | 0.42              |
| 1:E:256:ILE:HG21 | 1:E:259:ILE:HD12 | 2.01                     | 0.42              |
| 1:T:393:ALA:O    | 1:T:396:LEU:N    | 2.50                     | 0.42              |
| 1:U:344:ILE:O    | 1:U:344:ILE:HG22 | 2.19                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:17:ILE:CD1   | 1:U:65:GLU:HB3   | 2.47                     | 0.42              |
| 1:T:235:ILE:HG22 | 1:T:237:PRO:CD   | 2.48                     | 0.42              |
| 2:G:172:LEU:HA   | 2:G:172:LEU:HD23 | 1.70                     | 0.42              |
| 1:X:421:ILE:HG12 | 1:X:425:TYR:CD1  | 2.55                     | 0.42              |
| 1:X:37:ARG:HG3   | 1:X:48:VAL:HG11  | 2.01                     | 0.42              |
| 1:B:357:LYS:HA   | 1:B:367:ILE:HG23 | 2.01                     | 0.42              |
| 2:H:1:THR:CG2    | 2:H:33:LYS:HD3   | 2.49                     | 0.42              |
| 1:C:443:ILE:CG2  | 1:C:444:LEU:N    | 2.82                     | 0.42              |
| 1:S:35:TRP:C     | 1:S:37:ARG:N     | 2.72                     | 0.42              |
| 1:B:79:ILE:CG2   | 1:B:103:LEU:HD13 | 2.46                     | 0.42              |
| 1:A:369:PHE:CE2  | 1:A:421:ILE:HD12 | 2.55                     | 0.42              |
| 2:L:72:LEU:HD22  | 2:L:104:LEU:HD21 | 2.00                     | 0.42              |
| 2:O:52:ASP:HA    | 2:O:55:THR:OG1   | 2.20                     | 0.42              |
| 1:A:110:LEU:O    | 1:A:114:GLN:HB2  | 2.19                     | 0.42              |
| 1:F:321:PRO:O    | 1:F:322:GLU:C    | 2.57                     | 0.42              |
| 1:D:360:MET:CA   | 1:D:360:MET:HE2  | 2.50                     | 0.42              |
| 1:B:236:ASN:H    | 1:B:237:PRO:HD3  | 1.85                     | 0.42              |
| 1:F:235:ILE:O    | 1:F:236:ASN:CB   | 2.67                     | 0.42              |
| 2:I:60:PHE:CE2   | 2:I:97:VAL:HG11  | 2.54                     | 0.42              |
| 2:Q:154:ARG:O    | 2:Q:155:ILE:C    | 2.57                     | 0.42              |
| 2:J:73:LYS:O     | 2:J:74:SER:C     | 2.58                     | 0.42              |
| 2:G:19:GLN:OE1   | 2:G:21:SER:OG    | 2.38                     | 0.42              |
| 2:P:144:SER:OG   | 2:P:147:GLU:HB2  | 2.19                     | 0.42              |
| 1:B:398:THR:HG22 | 1:B:399:VAL:N    | 2.33                     | 0.42              |
| 1:A:51:LYS:HG3   | 1:F:401:GLU:OE1  | 2.19                     | 0.42              |
| 1:S:366:ASN:HA   | 1:S:366:ASN:HD22 | 1.63                     | 0.42              |
| 2:H:114:GLN:O    | 2:I:28:LYS:NZ    | 2.50                     | 0.42              |
| 1:W:240:LEU:N    | 1:W:240:LEU:HD12 | 2.34                     | 0.42              |
| 1:V:262:ILE:HD12 | 1:V:279:GLN:HB2  | 2.02                     | 0.42              |
| 1:V:279:GLN:HE22 | 1:V:319:LEU:CA   | 2.32                     | 0.42              |
| 1:C:52:ASN:ND2   | 1:C:305:PHE:CB   | 2.81                     | 0.42              |
| 1:X:439:LEU:C    | 1:X:441:ARG:H    | 2.22                     | 0.42              |
| 1:E:406:LYS:O    | 1:E:407:ILE:C    | 2.58                     | 0.42              |
| 2:Q:153:LEU:HB3  | 2:Q:167:PHE:CD2  | 2.54                     | 0.42              |
| 1:B:356:TYR:CE1  | 1:B:400:MET:HB3  | 2.54                     | 0.42              |
| 1:U:247:ALA:O    | 1:U:251:ASN:O    | 2.38                     | 0.42              |
| 1:D:37:ARG:O     | 1:D:38:MET:HB3   | 2.19                     | 0.42              |
| 1:U:437:GLU:O    | 1:U:437:GLU:HG3  | 2.20                     | 0.42              |
| 2:M:5:SER:CB     | 2:M:14:VAL:HG22  | 2.44                     | 0.42              |
| 1:U:235:ILE:C    | 1:U:237:PRO:HD3  | 2.40                     | 0.42              |
| 1:V:344:ILE:O    | 1:V:344:ILE:CG2  | 2.67                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:79:ILE:HG23  | 1:V:79:ILE:O     | 2.19                     | 0.42              |
| 1:C:34:ARG:NH2   | 1:C:253:ILE:CD1  | 2.82                     | 0.42              |
| 1:E:384:VAL:HG12 | 1:E:384:VAL:H    | 1.64                     | 0.42              |
| 1:V:15:GLN:O     | 1:V:349:HIS:N    | 2.50                     | 0.42              |
| 1:V:118:LYS:O    | 1:V:119:ASN:HB2  | 2.18                     | 0.42              |
| 2:N:78:LEU:O     | 2:N:81:ASP:HB2   | 2.19                     | 0.42              |
| 1:S:245:ILE:CG2  | 1:S:249:GLU:HG3  | 2.49                     | 0.42              |
| 1:C:42:GLU:HB3   | 1:C:43:PRO:HD3   | 2.00                     | 0.42              |
| 2:M:7:ARG:NH2    | 2:M:102:GLU:O    | 2.53                     | 0.42              |
| 1:X:262:ILE:HD12 | 1:X:279:GLN:HB2  | 2.02                     | 0.42              |
| 1:B:403:LEU:HD23 | 1:B:404:MET:CA   | 2.49                     | 0.42              |
| 2:M:164:ASN:ND2  | 2:M:164:ASN:N    | 2.56                     | 0.42              |
| 1:A:5:THR:O      | 1:A:6:PRO:C      | 2.58                     | 0.42              |
| 2:G:1:THR:CG2    | 2:G:33:LYS:NZ    | 2.82                     | 0.42              |
| 1:D:27:VAL:HB    | 1:D:70:LEU:CD2   | 2.41                     | 0.42              |
| 1:V:300:THR:O    | 1:V:302:HIS:N    | 2.52                     | 0.42              |
| 1:S:13:LEU:C     | 1:S:15:GLN:H     | 2.23                     | 0.42              |
| 1:B:443:ILE:HG22 | 1:B:444:LEU:N    | 2.34                     | 0.42              |
| 1:V:66:ILE:O     | 1:V:66:ILE:HG22  | 2.20                     | 0.42              |
| 1:T:36:ARG:NE    | 1:T:36:ARG:HA    | 2.33                     | 0.42              |
| 1:X:345:LEU:HD13 | 1:X:396:LEU:HD22 | 2.01                     | 0.42              |
| 1:X:341:PHE:CB   | 1:X:378:ALA:HB1  | 2.49                     | 0.42              |
| 2:H:60:PHE:HZ    | 2:H:71:LEU:HD22  | 1.84                     | 0.42              |
| 1:C:12:GLU:HG2   | 1:C:73:LEU:HD22  | 2.02                     | 0.42              |
| 1:U:28:ALA:C     | 1:U:30:ALA:N     | 2.72                     | 0.42              |
| 1:C:410:SER:O    | 1:C:411:ALA:C    | 2.58                     | 0.42              |
| 2:R:92:GLU:O     | 2:R:93:ALA:HB2   | 2.20                     | 0.42              |
| 1:B:394:ARG:HD3  | 1:B:394:ARG:HA   | 1.83                     | 0.42              |
| 1:W:441:ARG:HB3  | 1:W:442:PHE:HD1  | 1.85                     | 0.42              |
| 2:J:144:SER:CB   | 2:J:147:GLU:HG3  | 2.38                     | 0.42              |
| 1:U:35:TRP:C     | 1:U:37:ARG:N     | 2.73                     | 0.42              |
| 2:M:149:VAL:O    | 2:M:153:LEU:HG   | 2.19                     | 0.42              |
| 1:W:368:ALA:HB3  | 1:W:420:ASN:HA   | 2.02                     | 0.42              |
| 1:E:283:LEU:CB   | 1:E:284:PRO:CD   | 2.98                     | 0.42              |
| 1:D:38:MET:HG3   | 1:D:45:ARG:HH12  | 1.83                     | 0.42              |
| 1:D:356:TYR:O    | 1:D:357:LYS:C    | 2.56                     | 0.42              |
| 1:C:9:ILE:HD13   | 1:C:31:LEU:HD23  | 2.01                     | 0.42              |
| 1:B:434:VAL:O    | 1:B:435:GLU:HB2  | 2.19                     | 0.42              |
| 2:L:105:ILE:HG22 | 2:L:113:VAL:O    | 2.19                     | 0.42              |
| 2:O:4:VAL:HG12   | 2:O:153:LEU:CD2  | 2.50                     | 0.42              |
| 1:W:68:ARG:C     | 1:W:70:LEU:H     | 2.23                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:68:ARG:C     | 1:X:70:LEU:H     | 2.23                     | 0.42              |
| 1:U:48:VAL:HG22  | 1:U:48:VAL:O     | 2.20                     | 0.42              |
| 2:H:131:LEU:O    | 2:H:132:SER:C    | 2.58                     | 0.42              |
| 1:X:434:VAL:HG12 | 1:X:435:GLU:N    | 2.35                     | 0.42              |
| 1:U:28:ALA:O     | 1:U:30:ALA:N     | 2.52                     | 0.42              |
| 2:Q:71:LEU:O     | 2:Q:73:LYS:N     | 2.52                     | 0.42              |
| 1:F:382:PHE:HD2  | 1:F:382:PHE:C    | 2.24                     | 0.42              |
| 1:W:66:ILE:HG22  | 1:W:66:ILE:O     | 2.20                     | 0.42              |
| 1:C:52:ASN:HB2   | 1:C:326:ARG:O    | 2.20                     | 0.42              |
| 1:E:240:LEU:O    | 1:E:241:LYS:C    | 2.59                     | 0.42              |
| 1:U:357:LYS:HA   | 1:U:367:ILE:CD1  | 2.31                     | 0.42              |
| 1:T:64:THR:OG1   | 1:T:255:PHE:HE2  | 2.03                     | 0.42              |
| 2:P:153:LEU:HB3  | 2:P:167:PHE:CD2  | 2.55                     | 0.42              |
| 1:S:359:LEU:HD11 | 1:X:48:VAL:CG2   | 2.49                     | 0.42              |
| 2:H:82:TRP:CD1   | 2:H:88:LEU:HB2   | 2.55                     | 0.42              |
| 1:B:369:PHE:CE2  | 1:B:421:ILE:HD12 | 2.53                     | 0.42              |
| 1:E:293:THR:C    | 1:E:295:HIS:N    | 2.73                     | 0.42              |
| 2:O:42:VAL:HG21  | 2:O:64:LEU:CD1   | 2.50                     | 0.42              |
| 1:C:4:MET:HE2    | 1:C:9:ILE:HA     | 2.01                     | 0.42              |
| 1:F:86:PHE:HB2   | 1:F:278:VAL:HG13 | 2.01                     | 0.42              |
| 1:U:120:ARG:NH2  | 1:U:235:ILE:H    | 2.18                     | 0.42              |
| 2:H:72:LEU:HD13  | 2:H:72:LEU:O     | 2.19                     | 0.42              |
| 1:V:17:ILE:CD1   | 1:V:65:GLU:HB3   | 2.49                     | 0.42              |
| 1:U:341:PHE:CB   | 1:U:378:ALA:HB1  | 2.49                     | 0.42              |
| 1:T:61:VAL:HG12  | 1:T:336:LEU:HG   | 2.02                     | 0.42              |
| 1:T:51:LYS:HE2   | 1:U:356:TYR:OH   | 2.20                     | 0.42              |
| 1:T:351:SER:O    | 1:T:355:GLN:HG3  | 2.20                     | 0.42              |
| 2:K:6:VAL:CG1    | 2:K:7:ARG:N      | 2.83                     | 0.42              |
| 1:D:396:LEU:HA   | 1:D:396:LEU:HD23 | 1.83                     | 0.42              |
| 1:F:343:ARG:O    | 1:F:348:PRO:HD3  | 2.20                     | 0.42              |
| 2:N:43:LEU:HD11  | 2:N:172:LEU:HG   | 2.01                     | 0.42              |
| 2:O:13:VAL:HG12  | 2:O:169:ILE:HG22 | 2.02                     | 0.42              |
| 1:F:380:ALA:O    | 1:F:384:VAL:HG12 | 2.20                     | 0.42              |
| 1:U:63:LYS:HB2   | 3:U:458:ATP:O2B  | 2.20                     | 0.42              |
| 1:C:264:LYS:NZ   | 1:C:319:LEU:HA   | 2.35                     | 0.42              |
| 1:E:111:VAL:HG12 | 1:E:240:LEU:HD11 | 2.02                     | 0.42              |
| 2:M:153:LEU:HB3  | 2:M:167:PHE:CD2  | 2.55                     | 0.42              |
| 1:S:55:MET:HE2   | 1:S:306:ILE:HG21 | 2.01                     | 0.42              |
| 2:H:137:LEU:O    | 2:H:141:THR:CG2  | 2.58                     | 0.42              |
| 2:N:133:ALA:O    | 2:N:136:ALA:HB3  | 2.19                     | 0.42              |
| 1:U:368:ALA:HB3  | 1:U:420:ASN:HA   | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:382:PHE:O    | 1:B:383:ARG:C    | 2.57                     | 0.42              |
| 2:N:83:ARG:HH21  | 2:N:111:ASP:HA   | 1.85                     | 0.42              |
| 2:H:96:ILE:HD11  | 2:H:123:ILE:HG23 | 2.01                     | 0.42              |
| 1:D:357:LYS:HA   | 1:D:367:ILE:HG23 | 2.02                     | 0.42              |
| 1:C:383:ARG:O    | 1:C:387:LYS:HG2  | 2.20                     | 0.42              |
| 1:E:250:GLN:HE21 | 1:E:250:GLN:CA   | 2.33                     | 0.42              |
| 1:F:394:ARG:HA   | 1:F:394:ARG:HD3  | 1.86                     | 0.42              |
| 2:N:5:SER:CB     | 2:N:14:VAL:HG22  | 2.45                     | 0.42              |
| 1:B:435:GLU:CG   | 1:B:436:ASN:N    | 2.80                     | 0.42              |
| 2:H:72:LEU:C     | 2:H:72:LEU:CD1   | 2.88                     | 0.42              |
| 1:T:341:PHE:CB   | 1:T:378:ALA:HB1  | 2.50                     | 0.42              |
| 1:F:34:ARG:NH2   | 1:F:251:ASN:HA   | 2.35                     | 0.42              |
| 1:S:68:ARG:C     | 1:S:70:LEU:H     | 2.23                     | 0.42              |
| 1:D:249:GLU:HG2  | 1:D:299:LYS:H    | 1.85                     | 0.42              |
| 1:X:436:ASN:O    | 1:X:437:GLU:C    | 2.58                     | 0.42              |
| 1:T:407:ILE:HG23 | 1:T:408:SER:N    | 2.35                     | 0.42              |
| 2:H:154:ARG:O    | 2:H:155:ILE:C    | 2.58                     | 0.42              |
| 2:N:75:ALA:O     | 2:N:78:LEU:HB3   | 2.19                     | 0.42              |
| 2:I:3:ILE:O      | 2:I:122:ALA:HA   | 2.20                     | 0.42              |
| 1:A:71:ALA:HB1   | 1:A:78:PHE:HB2   | 2.00                     | 0.42              |
| 1:V:53:ILE:HG12  | 1:V:329:ILE:HB   | 2.01                     | 0.42              |
| 1:D:323:LEU:O    | 1:D:325:GLY:N    | 2.53                     | 0.42              |
| 1:D:414:MET:HG2  | 1:D:414:MET:O    | 2.20                     | 0.42              |
| 1:U:283:LEU:CD1  | 1:U:322:GLU:HB3  | 2.50                     | 0.41              |
| 1:C:51:LYS:O     | 1:C:52:ASN:C     | 2.58                     | 0.41              |
| 2:O:90:LYS:C     | 2:O:91:LEU:HD12  | 2.39                     | 0.41              |
| 2:I:91:LEU:H     | 2:I:91:LEU:CD2   | 2.30                     | 0.41              |
| 2:G:1:THR:CG2    | 2:G:33:LYS:HD3   | 2.49                     | 0.41              |
| 1:X:300:THR:O    | 1:X:302:HIS:N    | 2.52                     | 0.41              |
| 1:U:353:THR:HG22 | 1:U:369:PHE:HD1  | 1.84                     | 0.41              |
| 1:E:79:ILE:HD12  | 1:E:80:LYS:N     | 2.34                     | 0.41              |
| 1:B:359:LEU:HD12 | 1:C:36:ARG:CB    | 2.50                     | 0.41              |
| 2:L:144:SER:HB3  | 2:L:147:GLU:CG   | 2.43                     | 0.41              |
| 1:V:55:MET:HE1   | 1:V:63:LYS:O     | 2.20                     | 0.41              |
| 2:G:136:ALA:HB1  | 2:M:137:LEU:HD13 | 2.01                     | 0.41              |
| 1:U:341:PHE:HB2  | 1:U:378:ALA:HB1  | 2.02                     | 0.41              |
| 2:L:7:ARG:CZ     | 2:L:12:VAL:CG2   | 2.98                     | 0.41              |
| 1:V:356:TYR:CD1  | 1:V:404:MET:HG3  | 2.55                     | 0.41              |
| 1:C:112:ARG:HH11 | 1:C:112:ARG:HG2  | 1.84                     | 0.41              |
| 1:F:330:ARG:HG3  | 1:F:330:ARG:NH1  | 2.35                     | 0.41              |
| 2:O:13:VAL:HG21  | 2:O:146:HIS:HA   | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:92:GLU:O     | 2:N:93:ALA:HB2   | 2.20                     | 0.41              |
| 2:J:133:ALA:HB1  | 2:J:155:ILE:HD12 | 2.01                     | 0.41              |
| 2:G:30:ASN:ND2   | 2:L:116:GLU:HG2  | 2.35                     | 0.41              |
| 1:A:55:MET:HE3   | 1:A:306:ILE:HG21 | 2.02                     | 0.41              |
| 1:X:53:ILE:HG12  | 1:X:329:ILE:HB   | 2.01                     | 0.41              |
| 1:W:391:ILE:H    | 1:W:391:ILE:HG12 | 1.58                     | 0.41              |
| 2:Q:96:ILE:O     | 2:Q:96:ILE:HG22  | 2.20                     | 0.41              |
| 1:E:333:LEU:N    | 1:E:333:LEU:HD12 | 2.35                     | 0.41              |
| 2:N:7:ARG:NH2    | 2:N:102:GLU:O    | 2.52                     | 0.41              |
| 1:V:319:LEU:O    | 1:V:324:GLN:NE2  | 2.53                     | 0.41              |
| 1:U:259:ILE:HG23 | 1:U:260:ASP:N    | 2.34                     | 0.41              |
| 1:T:283:LEU:N    | 1:T:284:PRO:CD   | 2.83                     | 0.41              |
| 1:B:341:PHE:HA   | 1:B:344:ILE:CG1  | 2.50                     | 0.41              |
| 2:R:7:ARG:NH2    | 2:R:102:GLU:O    | 2.53                     | 0.41              |
| 2:Q:16:GLY:O     | 2:Q:167:PHE:CB   | 2.68                     | 0.41              |
| 1:T:368:ALA:O    | 1:T:421:ILE:HB   | 2.20                     | 0.41              |
| 2:G:83:ARG:HG2   | 2:G:83:ARG:NH1   | 2.35                     | 0.41              |
| 2:L:136:ALA:HB1  | 2:R:137:LEU:HD13 | 2.02                     | 0.41              |
| 2:L:107:THR:OG1  | 2:L:111:ASP:OD2  | 2.24                     | 0.41              |
| 1:W:300:THR:O    | 1:W:302:HIS:N    | 2.53                     | 0.41              |
| 1:W:35:TRP:C     | 1:W:37:ARG:N     | 2.73                     | 0.41              |
| 1:X:6:PRO:C      | 1:X:8:GLU:N      | 2.74                     | 0.41              |
| 1:C:421:ILE:HA   | 1:C:425:TYR:CD1  | 2.49                     | 0.41              |
| 1:W:336:LEU:HB2  | 1:W:341:PHE:CE1  | 2.55                     | 0.41              |
| 1:T:13:LEU:C     | 1:T:15:GLN:H     | 2.24                     | 0.41              |
| 1:D:112:ARG:O    | 1:D:114:GLN:N    | 2.53                     | 0.41              |
| 2:O:13:VAL:HG13  | 2:O:171:GLU:HB3  | 2.02                     | 0.41              |
| 1:D:42:GLU:HB3   | 1:D:43:PRO:HD3   | 2.02                     | 0.41              |
| 1:A:353:THR:O    | 1:A:354:GLU:C    | 2.58                     | 0.41              |
| 1:F:53:ILE:O     | 1:F:306:ILE:HA   | 2.20                     | 0.41              |
| 1:U:390:ASN:HD22 | 1:U:390:ASN:C    | 2.24                     | 0.41              |
| 1:A:395:ARG:HA   | 1:A:395:ARG:HD3  | 1.89                     | 0.41              |
| 1:D:264:LYS:HZ1  | 1:D:319:LEU:HA   | 1.85                     | 0.41              |
| 1:B:232:ALA:H    | 1:B:234:LEU:HD21 | 1.83                     | 0.41              |
| 1:C:393:ALA:HB3  | 3:C:452:ATP:C8   | 2.55                     | 0.41              |
| 2:P:90:LYS:C     | 2:P:91:LEU:HD12  | 2.40                     | 0.41              |
| 2:K:83:ARG:HG2   | 2:L:55:THR:HB    | 2.02                     | 0.41              |
| 2:N:153:LEU:HB3  | 2:N:167:PHE:CE2  | 2.54                     | 0.41              |
| 1:X:48:VAL:HG22  | 1:X:48:VAL:O     | 2.19                     | 0.41              |
| 2:G:77:GLU:OE2   | 2:G:80:LYS:HD2   | 2.19                     | 0.41              |
| 1:C:36:ARG:O     | 1:C:39:GLN:CB    | 2.64                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:78:LEU:HG    | 2:G:82:TRP:HZ3   | 1.85                     | 0.41              |
| 1:V:64:THR:OG1   | 1:V:255:PHE:HE2  | 2.04                     | 0.41              |
| 1:T:117:ALA:O    | 1:T:121:ALA:N    | 2.53                     | 0.41              |
| 1:E:76:ALA:HB1   | 1:E:251:ASN:O    | 2.20                     | 0.41              |
| 1:D:256:ILE:O    | 1:D:256:ILE:HG22 | 2.20                     | 0.41              |
| 1:F:240:LEU:O    | 1:F:241:LYS:C    | 2.58                     | 0.41              |
| 1:E:311:PHE:CE1  | 1:E:316:PRO:HA   | 2.55                     | 0.41              |
| 1:B:428:ASP:O    | 1:B:431:GLY:N    | 2.51                     | 0.41              |
| 2:H:172:LEU:HA   | 2:H:173:PRO:HD2  | 1.98                     | 0.41              |
| 2:N:71:LEU:O     | 2:N:73:LYS:N     | 2.53                     | 0.41              |
| 1:F:244:ALA:O    | 1:F:247:ALA:HB3  | 2.19                     | 0.41              |
| 2:G:129:TYR:N    | 2:G:129:TYR:CD2  | 2.88                     | 0.41              |
| 2:M:96:ILE:O     | 2:M:96:ILE:HG22  | 2.20                     | 0.41              |
| 1:X:441:ARG:HB3  | 1:X:442:PHE:H    | 1.70                     | 0.41              |
| 1:E:351:SER:O    | 1:E:355:GLN:HG3  | 2.21                     | 0.41              |
| 1:E:421:ILE:HA   | 1:E:425:TYR:CD1  | 2.45                     | 0.41              |
| 2:Q:134:ALA:O    | 2:Q:137:LEU:N    | 2.54                     | 0.41              |
| 1:D:71:ALA:HB1   | 1:D:78:PHE:HB2   | 2.02                     | 0.41              |
| 2:J:46:PHE:HB3   | 2:J:95:LEU:HD21  | 2.03                     | 0.41              |
| 1:X:393:ALA:CB   | 3:X:461:ATP:H1'  | 2.51                     | 0.41              |
| 1:T:35:TRP:C     | 1:T:37:ARG:N     | 2.73                     | 0.41              |
| 1:E:61:VAL:HA    | 1:E:336:LEU:HD22 | 2.02                     | 0.41              |
| 1:S:9:ILE:O      | 1:S:13:LEU:HG    | 2.21                     | 0.41              |
| 1:B:245:ILE:O    | 1:B:246:ASP:C    | 2.57                     | 0.41              |
| 1:U:79:ILE:O     | 1:U:79:ILE:HG23  | 2.20                     | 0.41              |
| 2:O:4:VAL:HA     | 2:O:121:LEU:O    | 2.20                     | 0.41              |
| 2:L:7:ARG:NH2    | 2:L:12:VAL:HG21  | 2.35                     | 0.41              |
| 1:A:21:ALA:O     | 1:A:22:ASP:C     | 2.57                     | 0.41              |
| 1:E:428:ASP:O    | 1:E:430:LEU:N    | 2.54                     | 0.41              |
| 1:F:414:MET:O    | 1:F:414:MET:HG2  | 2.20                     | 0.41              |
| 2:Q:32:ARG:HH11  | 2:Q:32:ARG:HG3   | 1.86                     | 0.41              |
| 2:I:172:LEU:HA   | 2:I:172:LEU:HD23 | 1.74                     | 0.41              |
| 1:T:390:ASN:C    | 1:T:390:ASN:HD22 | 2.24                     | 0.41              |
| 1:S:279:GLN:HE22 | 1:S:319:LEU:CA   | 2.33                     | 0.41              |
| 1:D:403:LEU:HD23 | 1:D:404:MET:CA   | 2.51                     | 0.41              |
| 1:U:54:LEU:HD11  | 1:U:327:LEU:HB3  | 2.02                     | 0.41              |
| 2:R:134:ALA:O    | 2:R:135:ARG:C    | 2.59                     | 0.41              |
| 1:E:71:ALA:CB    | 1:E:78:PHE:HB2   | 2.51                     | 0.41              |
| 1:E:344:ILE:HG23 | 3:E:454:ATP:C2   | 2.55                     | 0.41              |
| 2:K:105:ILE:O    | 2:K:105:ILE:HG23 | 2.21                     | 0.41              |
| 2:Q:64:LEU:HD23  | 2:Q:64:LEU:HA    | 1.96                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:367:ILE:CD1  | 1:C:421:ILE:HD11 | 2.51                     | 0.41              |
| 1:C:38:MET:HA    | 1:C:45:ARG:HH11  | 1.86                     | 0.41              |
| 1:B:256:ILE:HD13 | 1:B:282:LEU:HD13 | 2.02                     | 0.41              |
| 1:D:300:THR:HA   | 1:D:303:ILE:HG12 | 2.03                     | 0.41              |
| 1:S:61:VAL:HG12  | 1:S:336:LEU:HG   | 2.02                     | 0.41              |
| 1:E:55:MET:C     | 1:E:56:ILE:HD12  | 2.41                     | 0.41              |
| 2:O:149:VAL:O    | 2:O:153:LEU:HG   | 2.21                     | 0.41              |
| 2:R:157:GLY:HA2  | 2:R:163:THR:CG2  | 2.50                     | 0.41              |
| 1:W:407:ILE:HG23 | 1:W:408:SER:N    | 2.36                     | 0.41              |
| 1:T:356:TYR:CD1  | 1:T:404:MET:HG3  | 2.56                     | 0.41              |
| 2:O:82:TRP:CE3   | 2:O:110:GLY:HA2  | 2.55                     | 0.41              |
| 2:O:127:GLY:O    | 2:O:129:TYR:N    | 2.53                     | 0.41              |
| 1:B:69:ARG:O     | 1:B:70:LEU:C     | 2.58                     | 0.41              |
| 2:N:104:LEU:HD13 | 2:N:112:VAL:HG11 | 2.00                     | 0.41              |
| 2:I:7:ARG:HD2    | 2:I:119:GLN:CD   | 2.32                     | 0.41              |
| 1:F:403:LEU:HB2  | 1:F:430:LEU:HD21 | 2.01                     | 0.41              |
| 1:U:55:MET:HE1   | 1:U:63:LYS:O     | 2.21                     | 0.41              |
| 2:O:91:LEU:HB2   | 2:O:108:GLY:HA3  | 2.03                     | 0.41              |
| 2:H:83:ARG:HD3   | 2:I:54:PHE:CB    | 2.49                     | 0.41              |
| 2:N:17:ASP:OD2   | 2:N:33:LYS:HE3   | 2.20                     | 0.41              |
| 1:B:4:MET:CE     | 1:B:9:ILE:HA     | 2.51                     | 0.41              |
| 2:H:78:LEU:HD12  | 2:H:78:LEU:O     | 2.20                     | 0.41              |
| 1:U:369:PHE:HE2  | 1:U:421:ILE:CD1  | 2.22                     | 0.41              |
| 2:K:164:ASN:HD22 | 2:K:164:ASN:C    | 2.24                     | 0.41              |
| 1:T:300:THR:O    | 1:T:301:ASP:C    | 2.59                     | 0.41              |
| 1:E:105:ASP:O    | 1:E:108:MET:HB2  | 2.21                     | 0.41              |
| 2:O:104:LEU:HD13 | 2:O:112:VAL:HG11 | 2.02                     | 0.41              |
| 2:O:7:ARG:NH2    | 2:O:102:GLU:O    | 2.53                     | 0.41              |
| 1:A:100:ILE:HG22 | 1:A:298:VAL:HG21 | 2.01                     | 0.41              |
| 1:T:385:ASN:ND2  | 1:T:395:ARG:HE   | 2.14                     | 0.41              |
| 1:D:321:PRO:O    | 1:D:322:GLU:C    | 2.59                     | 0.41              |
| 1:S:345:LEU:HD21 | 1:S:377:ILE:HG22 | 2.03                     | 0.41              |
| 1:F:31:LEU:HD12  | 1:F:31:LEU:O     | 2.21                     | 0.41              |
| 1:F:260:ASP:HB3  | 1:F:311:PHE:CD2  | 2.55                     | 0.41              |
| 1:D:112:ARG:C    | 1:D:114:GLN:N    | 2.74                     | 0.41              |
| 1:A:390:ASN:C    | 1:A:390:ASN:OD1  | 2.59                     | 0.41              |
| 2:I:44:ALA:HA    | 2:I:96:ILE:O     | 2.20                     | 0.41              |
| 1:F:300:THR:HA   | 1:F:303:ILE:HG12 | 2.03                     | 0.41              |
| 1:T:49:THR:HA    | 1:T:50:PRO:HD3   | 1.95                     | 0.41              |
| 2:L:134:ALA:O    | 2:L:135:ARG:C    | 2.59                     | 0.41              |
| 1:U:331:VAL:HG13 | 1:U:331:VAL:O    | 2.21                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:408:SER:O    | 1:E:36:ARG:NH2   | 2.46                     | 0.41              |
| 1:W:283:LEU:CD1  | 1:W:322:GLU:HB3  | 2.48                     | 0.41              |
| 2:G:2:THR:O      | 2:G:16:GLY:HA2   | 2.21                     | 0.41              |
| 2:K:72:LEU:O     | 2:K:72:LEU:HD13  | 2.19                     | 0.41              |
| 2:O:8:ARG:HH22   | 2:O:143:LEU:H    | 1.67                     | 0.41              |
| 1:B:367:ILE:HD11 | 1:B:421:ILE:CD1  | 2.49                     | 0.41              |
| 1:V:421:ILE:HG12 | 1:V:425:TYR:CE1  | 2.56                     | 0.41              |
| 1:V:48:VAL:O     | 1:V:48:VAL:HG22  | 2.20                     | 0.41              |
| 1:E:103:LEU:HD23 | 1:E:248:VAL:HG13 | 2.03                     | 0.41              |
| 1:S:300:THR:O    | 1:S:301:ASP:C    | 2.59                     | 0.41              |
| 1:E:341:PHE:HA   | 1:E:344:ILE:CG1  | 2.51                     | 0.41              |
| 1:D:116:ILE:HD12 | 1:D:117:ALA:CA   | 2.50                     | 0.41              |
| 1:D:32:ARG:NH1   | 1:D:35:TRP:CE3   | 2.89                     | 0.41              |
| 1:A:331:VAL:HG13 | 1:A:331:VAL:O    | 2.21                     | 0.41              |
| 1:C:57:GLY:CA    | 1:C:63:LYS:HE3   | 2.47                     | 0.41              |
| 1:C:20:GLN:OE1   | 1:C:333:LEU:HB3  | 2.21                     | 0.41              |
| 1:A:407:ILE:O    | 1:A:411:ALA:CB   | 2.69                     | 0.41              |
| 2:N:52:ASP:HA    | 2:N:55:THR:OG1   | 2.21                     | 0.41              |
| 1:C:253:ILE:HG23 | 1:C:304:LEU:HD23 | 2.01                     | 0.41              |
| 2:L:7:ARG:NH2    | 2:L:102:GLU:O    | 2.53                     | 0.41              |
| 1:U:356:TYR:CD1  | 1:U:404:MET:HG3  | 2.56                     | 0.41              |
| 1:S:387:LYS:HZ1  | 1:S:435:GLU:HG3  | 1.84                     | 0.41              |
| 2:O:154:ARG:O    | 2:O:155:ILE:C    | 2.59                     | 0.41              |
| 2:M:13:VAL:HG12  | 2:M:169:ILE:HG22 | 2.02                     | 0.41              |
| 2:M:78:LEU:O     | 2:M:81:ASP:HB2   | 2.21                     | 0.41              |
| 1:A:73:LEU:O     | 1:A:73:LEU:HD12  | 2.20                     | 0.41              |
| 1:T:437:GLU:CG   | 1:T:438:ASP:H    | 2.17                     | 0.41              |
| 2:M:76:VAL:CG1   | 1:S:442:PHE:CE2  | 3.04                     | 0.41              |
| 1:V:357:LYS:CA   | 1:V:367:ILE:HD11 | 2.34                     | 0.41              |
| 1:E:52:ASN:HD22  | 1:E:305:PHE:HB2  | 1.80                     | 0.41              |
| 2:O:164:ASN:ND2  | 2:O:164:ASN:N    | 2.59                     | 0.41              |
| 1:W:368:ALA:O    | 1:W:421:ILE:HB   | 2.21                     | 0.41              |
| 2:P:33:LYS:HA    | 2:P:46:PHE:CZ    | 2.55                     | 0.41              |
| 1:U:368:ALA:O    | 1:U:421:ILE:HB   | 2.21                     | 0.41              |
| 1:B:357:LYS:HG2  | 1:B:367:ILE:HG23 | 2.02                     | 0.41              |
| 1:A:235:ILE:HG22 | 1:A:237:PRO:N    | 2.36                     | 0.41              |
| 2:L:1:THR:HG23   | 2:L:33:LYS:CE    | 2.51                     | 0.41              |
| 1:F:17:ILE:HG12  | 1:F:66:ILE:CG1   | 2.51                     | 0.41              |
| 1:V:353:THR:HG22 | 1:V:369:PHE:HD1  | 1.82                     | 0.41              |
| 1:D:57:GLY:CA    | 1:D:63:LYS:HE3   | 2.50                     | 0.41              |
| 2:H:44:ALA:HA    | 2:H:96:ILE:O     | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:46:PHE:O     | 2:K:46:PHE:CD2   | 2.73                     | 0.41              |
| 1:A:326:ARG:HD2  | 1:F:394:ARG:NH2  | 2.35                     | 0.41              |
| 1:A:100:ILE:CG2  | 1:A:298:VAL:HG21 | 2.51                     | 0.41              |
| 1:X:341:PHE:HB2  | 1:X:378:ALA:HB1  | 2.03                     | 0.41              |
| 1:X:345:LEU:HD21 | 1:X:377:ILE:HG22 | 2.03                     | 0.41              |
| 1:V:18:ILE:CG2   | 1:V:344:ILE:HG13 | 2.50                     | 0.41              |
| 1:B:407:ILE:O    | 1:B:411:ALA:CB   | 2.68                     | 0.41              |
| 1:A:54:LEU:HG    | 1:A:56:ILE:HD12  | 2.02                     | 0.41              |
| 1:B:34:ARG:NH2   | 1:B:253:ILE:HD13 | 2.36                     | 0.41              |
| 1:D:384:VAL:O    | 1:D:387:LYS:N    | 2.53                     | 0.41              |
| 2:P:154:ARG:O    | 2:P:155:ILE:C    | 2.58                     | 0.41              |
| 1:V:265:LYS:H    | 1:V:269:SER:CB   | 2.34                     | 0.41              |
| 1:F:353:THR:O    | 1:F:354:GLU:C    | 2.57                     | 0.41              |
| 1:B:25:ARG:O     | 1:B:28:ALA:HB3   | 2.21                     | 0.41              |
| 1:A:263:CYS:C    | 1:A:264:LYS:HE3  | 2.40                     | 0.41              |
| 1:V:259:ILE:HG23 | 1:V:260:ASP:N    | 2.36                     | 0.41              |
| 1:W:331:VAL:HG13 | 1:W:331:VAL:O    | 2.20                     | 0.41              |
| 1:U:65:GLU:HG3   | 3:U:458:ATP:H2'  | 2.03                     | 0.41              |
| 1:B:336:LEU:HA   | 1:B:336:LEU:HD12 | 1.65                     | 0.41              |
| 2:G:164:ASN:HD22 | 2:G:164:ASN:H    | 1.69                     | 0.41              |
| 2:N:153:LEU:HB3  | 2:N:167:PHE:CD2  | 2.56                     | 0.41              |
| 1:S:54:LEU:HD23  | 1:S:307:ALA:HB3  | 2.01                     | 0.41              |
| 1:S:55:MET:HE3   | 1:S:255:PHE:HE1  | 1.84                     | 0.41              |
| 2:K:51:ALA:O     | 2:K:52:ASP:C     | 2.58                     | 0.41              |
| 1:B:380:ALA:O    | 1:B:383:ARG:HB3  | 2.21                     | 0.41              |
| 1:V:54:LEU:HD23  | 1:V:307:ALA:HB3  | 2.03                     | 0.41              |
| 1:D:78:PHE:HD1   | 1:D:253:ILE:HB   | 1.85                     | 0.41              |
| 2:P:131:LEU:HD12 | 2:P:135:ARG:HG3  | 2.03                     | 0.41              |
| 1:F:17:ILE:HB    | 1:F:24:LYS:HE3   | 2.02                     | 0.41              |
| 1:V:373:ALA:CB   | 1:V:422:ASP:HA   | 2.50                     | 0.41              |
| 1:V:48:VAL:HA    | 1:W:355:GLN:OE1  | 2.21                     | 0.41              |
| 2:J:115:PRO:CB   | 2:J:119:GLN:HA   | 2.51                     | 0.41              |
| 1:D:245:ILE:HG23 | 1:D:298:VAL:HG12 | 2.02                     | 0.41              |
| 1:E:104:THR:OG1  | 1:E:293:THR:HG21 | 2.20                     | 0.41              |
| 1:E:336:LEU:HD12 | 1:E:336:LEU:HA   | 1.77                     | 0.41              |
| 1:E:344:ILE:HG12 | 1:E:344:ILE:H    | 1.58                     | 0.41              |
| 1:S:6:PRO:C      | 1:S:8:GLU:N      | 2.73                     | 0.41              |
| 1:S:326:ARG:HA   | 1:S:326:ARG:HD2  | 1.96                     | 0.41              |
| 1:B:100:ILE:HG22 | 1:B:298:VAL:HG21 | 2.02                     | 0.41              |
| 1:C:369:PHE:CE2  | 1:C:421:ILE:HD12 | 2.55                     | 0.41              |
| 1:B:438:ASP:CG   | 1:B:439:LEU:N    | 2.75                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:37:ARG:HH12  | 1:B:38:MET:HE2   | 1.86                     | 0.41              |
| 2:K:91:LEU:HD12  | 2:K:91:LEU:HA    | 1.82                     | 0.41              |
| 1:X:15:GLN:O     | 1:X:348:PRO:HA   | 2.20                     | 0.41              |
| 1:D:100:ILE:HG13 | 1:D:300:THR:CG2  | 2.51                     | 0.41              |
| 1:D:341:PHE:HA   | 1:D:344:ILE:HG12 | 2.02                     | 0.41              |
| 1:D:343:ARG:C    | 1:D:345:LEU:N    | 2.73                     | 0.41              |
| 1:X:73:LEU:HD12  | 1:X:73:LEU:N     | 2.36                     | 0.41              |
| 1:A:34:ARG:HH22  | 1:A:253:ILE:HD13 | 1.85                     | 0.41              |
| 2:K:88:LEU:O     | 2:K:89:ARG:O     | 2.37                     | 0.41              |
| 1:F:235:ILE:O    | 1:F:236:ASN:HB3  | 2.21                     | 0.41              |
| 1:V:407:ILE:HG23 | 1:V:408:SER:N    | 2.36                     | 0.41              |
| 1:A:341:PHE:HA   | 1:A:344:ILE:HG12 | 2.02                     | 0.41              |
| 1:B:410:SER:C    | 1:B:412:SER:N    | 2.74                     | 0.41              |
| 2:K:131:LEU:HD21 | 2:K:135:ARG:NH2  | 2.36                     | 0.41              |
| 1:S:387:LYS:NZ   | 1:S:435:GLU:CG   | 2.84                     | 0.41              |
| 2:J:7:ARG:HA     | 2:J:11:GLN:O     | 2.20                     | 0.41              |
| 2:O:32:ARG:HG3   | 2:O:32:ARG:HH11  | 1.86                     | 0.41              |
| 2:K:98:ALA:CB    | 2:K:103:SER:HA   | 2.50                     | 0.41              |
| 1:A:384:VAL:O    | 1:A:385:ASN:C    | 2.58                     | 0.41              |
| 1:E:98:SER:O     | 1:E:99:ILE:C     | 2.59                     | 0.41              |
| 1:E:282:LEU:O    | 1:E:285:LEU:HB2  | 2.21                     | 0.41              |
| 2:J:24:ASN:O     | 2:O:161:VAL:HG13 | 2.21                     | 0.41              |
| 2:R:82:TRP:CE3   | 2:R:110:GLY:HA2  | 2.56                     | 0.41              |
| 1:C:313:VAL:HG23 | 1:C:314:ALA:H    | 1.85                     | 0.41              |
| 2:I:161:VAL:HG13 | 2:N:24:ASN:O     | 2.21                     | 0.41              |
| 2:N:96:ILE:HG22  | 2:N:96:ILE:O     | 2.20                     | 0.41              |
| 2:I:115:PRO:HG3  | 2:I:121:LEU:HD11 | 2.03                     | 0.41              |
| 2:J:1:THR:HG22   | 2:J:2:THR:H      | 1.85                     | 0.41              |
| 2:Q:4:VAL:HG12   | 2:Q:153:LEU:CD2  | 2.50                     | 0.41              |
| 2:N:153:LEU:HD23 | 2:N:153:LEU:HA   | 1.90                     | 0.41              |
| 1:E:443:ILE:HG22 | 1:E:444:LEU:N    | 2.35                     | 0.41              |
| 1:B:105:ASP:O    | 1:B:108:MET:HB2  | 2.21                     | 0.41              |
| 1:S:331:VAL:O    | 1:S:331:VAL:HG13 | 2.21                     | 0.41              |
| 2:I:1:THR:HG23   | 2:I:33:LYS:HD3   | 2.03                     | 0.41              |
| 2:K:164:ASN:ND2  | 2:K:164:ASN:H    | 2.18                     | 0.41              |
| 2:P:134:ALA:O    | 2:P:135:ARG:C    | 2.59                     | 0.41              |
| 1:X:17:ILE:CD1   | 1:X:66:ILE:HG12  | 2.51                     | 0.41              |
| 1:D:37:ARG:O     | 1:D:38:MET:CB    | 2.67                     | 0.41              |
| 2:H:6:VAL:CG1    | 2:H:7:ARG:N      | 2.84                     | 0.41              |
| 1:E:250:GLN:HE21 | 1:E:250:GLN:HA   | 1.86                     | 0.41              |
| 1:C:31:LEU:HD21  | 1:C:74:ALA:HB2   | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:43:LEU:O     | 2:Q:97:VAL:HA    | 2.21                     | 0.41              |
| 2:I:134:ALA:O    | 2:I:138:VAL:HG23 | 2.20                     | 0.41              |
| 2:P:20:VAL:CG2   | 1:W:444:LEU:HD21 | 2.51                     | 0.41              |
| 2:J:6:VAL:HG12   | 2:J:7:ARG:N      | 2.35                     | 0.41              |
| 2:H:155:ILE:O    | 2:H:159:ILE:HG13 | 2.21                     | 0.41              |
| 1:T:265:LYS:H    | 1:T:269:SER:CB   | 2.33                     | 0.41              |
| 1:T:53:ILE:HG12  | 1:T:329:ILE:HB   | 2.02                     | 0.41              |
| 1:F:426:VAL:O    | 1:F:427:ALA:C    | 2.59                     | 0.41              |
| 2:G:24:ASN:O     | 2:R:161:VAL:HG22 | 2.21                     | 0.41              |
| 2:I:70:HIS:O     | 2:I:71:LEU:C     | 2.60                     | 0.41              |
| 2:I:49:GLY:O     | 2:I:50:THR:C     | 2.60                     | 0.41              |
| 2:L:73:LYS:O     | 2:L:74:SER:C     | 2.57                     | 0.41              |
| 1:S:69:ARG:HH11  | 1:S:69:ARG:HG2   | 1.85                     | 0.41              |
| 1:W:439:LEU:O    | 1:W:440:SER:C    | 2.59                     | 0.40              |
| 1:F:381:ALA:O    | 1:F:382:PHE:C    | 2.60                     | 0.40              |
| 1:W:283:LEU:HD21 | 1:W:322:GLU:HG2  | 2.02                     | 0.40              |
| 1:E:362:THR:HG21 | 1:F:39:GLN:HG2   | 2.01                     | 0.40              |
| 1:T:421:ILE:HG12 | 1:T:425:TYR:CD1  | 2.56                     | 0.40              |
| 1:S:17:ILE:HG23  | 3:S:456:ATP:HN61 | 1.85                     | 0.40              |
| 2:P:17:ASP:C     | 2:P:33:LYS:HD2   | 2.42                     | 0.40              |
| 2:J:99:ASP:HA    | 2:J:172:LEU:CD1  | 2.51                     | 0.40              |
| 1:X:20:GLN:O     | 1:X:21:ALA:CB    | 2.67                     | 0.40              |
| 1:D:108:MET:HE2  | 1:D:241:LYS:HA   | 2.02                     | 0.40              |
| 1:X:260:ASP:HB3  | 1:X:311:PHE:HD2  | 1.76                     | 0.40              |
| 1:A:48:VAL:HA    | 1:F:355:GLN:OE1  | 2.21                     | 0.40              |
| 2:O:64:LEU:HD23  | 2:O:64:LEU:HA    | 1.94                     | 0.40              |
| 1:B:416:GLY:O    | 1:B:417:GLN:O    | 2.39                     | 0.40              |
| 1:D:111:VAL:HG21 | 1:D:244:ALA:N    | 2.36                     | 0.40              |
| 2:L:4:VAL:HG23   | 2:L:122:ALA:HB2  | 2.03                     | 0.40              |
| 2:J:49:GLY:O     | 2:J:50:THR:C     | 2.59                     | 0.40              |
| 1:C:115:GLU:C    | 1:C:117:ALA:H    | 2.23                     | 0.40              |
| 1:S:441:ARG:HD3  | 1:S:441:ARG:HA   | 1.80                     | 0.40              |
| 1:U:262:ILE:HD12 | 1:U:279:GLN:HB2  | 2.03                     | 0.40              |
| 1:T:322:GLU:HG3  | 1:U:394:ARG:HH12 | 1.86                     | 0.40              |
| 1:E:52:ASN:HD21  | 1:E:305:PHE:H    | 1.55                     | 0.40              |
| 1:E:360:MET:HE3  | 1:F:36:ARG:NH1   | 2.36                     | 0.40              |
| 2:G:1:THR:HG23   | 2:G:33:LYS:HD3   | 2.03                     | 0.40              |
| 1:A:436:ASN:HB3  | 1:A:439:LEU:HD12 | 2.03                     | 0.40              |
| 1:B:241:LYS:HD3  | 1:B:295:HIS:HA   | 2.03                     | 0.40              |
| 2:P:115:PRO:HG3  | 2:P:121:LEU:HG   | 2.03                     | 0.40              |
| 2:H:82:TRP:CE2   | 2:H:108:GLY:O    | 2.74                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:172:LEU:HA   | 2:J:172:LEU:HD23 | 1.78                     | 0.40              |
| 2:J:42:VAL:HG21  | 2:J:64:LEU:HD13  | 2.02                     | 0.40              |
| 1:X:18:ILE:HG22  | 1:X:344:ILE:CG1  | 2.51                     | 0.40              |
| 1:V:37:ARG:HG3   | 1:V:48:VAL:HG11  | 2.03                     | 0.40              |
| 1:E:78:PHE:CD2   | 1:E:79:ILE:N     | 2.89                     | 0.40              |
| 1:W:13:LEU:C     | 1:W:15:GLN:H     | 2.24                     | 0.40              |
| 1:F:19:GLY:O     | 1:F:20:GLN:C     | 2.58                     | 0.40              |
| 1:E:10:VAL:O     | 1:E:11:SER:C     | 2.60                     | 0.40              |
| 1:F:86:PHE:CE2   | 1:F:96:VAL:HA    | 2.56                     | 0.40              |
| 1:V:6:PRO:C      | 1:V:8:GLU:N      | 2.74                     | 0.40              |
| 1:D:340:ASP:O    | 1:D:344:ILE:HD11 | 2.22                     | 0.40              |
| 1:F:321:PRO:HA   | 1:F:324:GLN:HB3  | 2.02                     | 0.40              |
| 1:C:407:ILE:CD1  | 1:C:419:VAL:HG11 | 2.51                     | 0.40              |
| 2:G:71:LEU:C     | 2:G:71:LEU:CD1   | 2.89                     | 0.40              |
| 1:T:68:ARG:C     | 1:T:70:LEU:H     | 2.24                     | 0.40              |
| 1:D:54:LEU:HG    | 1:D:56:ILE:CD1   | 2.51                     | 0.40              |
| 1:C:360:MET:HE1  | 1:C:360:MET:HA   | 2.03                     | 0.40              |
| 1:D:323:LEU:C    | 1:D:325:GLY:N    | 2.75                     | 0.40              |
| 2:R:54:PHE:HA    | 2:R:57:PHE:HB3   | 2.04                     | 0.40              |
| 1:C:339:ALA:O    | 1:C:342:GLU:HB2  | 2.22                     | 0.40              |
| 2:M:54:PHE:HA    | 2:M:57:PHE:HB3   | 2.03                     | 0.40              |
| 1:E:435:GLU:OE1  | 1:E:435:GLU:N    | 2.54                     | 0.40              |
| 1:T:366:ASN:HA   | 1:T:366:ASN:HD22 | 1.63                     | 0.40              |
| 2:M:112:VAL:O    | 1:S:444:LEU:HD13 | 2.22                     | 0.40              |
| 1:U:283:LEU:HD21 | 1:U:322:GLU:HG2  | 2.04                     | 0.40              |
| 2:R:7:ARG:CZ     | 2:R:12:VAL:CG2   | 2.99                     | 0.40              |
| 2:P:91:LEU:HB2   | 2:P:108:GLY:HA3  | 2.04                     | 0.40              |
| 2:Q:149:VAL:O    | 2:Q:153:LEU:HG   | 2.21                     | 0.40              |
| 1:V:370:THR:HG21 | 1:V:422:ASP:CB   | 2.51                     | 0.40              |
| 1:W:300:THR:O    | 1:W:301:ASP:C    | 2.60                     | 0.40              |
| 2:N:37:LEU:HD23  | 1:U:441:ARG:NH2  | 2.36                     | 0.40              |
| 1:A:262:ILE:HG21 | 1:A:262:ILE:HD13 | 1.85                     | 0.40              |
| 1:E:250:GLN:CA   | 1:E:250:GLN:NE2  | 2.84                     | 0.40              |
| 1:X:36:ARG:HE    | 1:X:36:ARG:CA    | 2.30                     | 0.40              |
| 1:E:416:GLY:O    | 1:E:417:GLN:O    | 2.40                     | 0.40              |
| 1:F:6:PRO:HD3    | 1:F:32:ARG:CD    | 2.51                     | 0.40              |
| 1:V:36:ARG:NE    | 1:V:36:ARG:HA    | 2.32                     | 0.40              |
| 2:J:60:PHE:HZ    | 2:J:71:LEU:HD22  | 1.87                     | 0.40              |
| 1:T:15:GLN:O     | 1:T:349:HIS:N    | 2.50                     | 0.40              |
| 1:U:265:LYS:H    | 1:U:269:SER:CB   | 2.33                     | 0.40              |
| 1:D:84:THR:C     | 1:D:86:PHE:H     | 2.24                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:75:ALA:O     | 2:M:78:LEU:HB3   | 2.21                     | 0.40              |
| 2:M:47:ALA:HB3   | 2:M:123:ILE:HD12 | 2.04                     | 0.40              |
| 2:H:67:HIS:CD2   | 2:H:73:LYS:HD3   | 2.56                     | 0.40              |
| 2:P:116:GLU:O    | 2:P:117:GLU:C    | 2.59                     | 0.40              |
| 2:P:78:LEU:O     | 2:P:81:ASP:HB2   | 2.20                     | 0.40              |
| 2:M:98:ALA:CB    | 2:M:103:SER:HA   | 2.52                     | 0.40              |
| 1:U:322:GLU:HG3  | 1:V:394:ARG:HH12 | 1.87                     | 0.40              |
| 1:T:279:GLN:O    | 1:T:320:ILE:HD11 | 2.21                     | 0.40              |
| 1:B:279:GLN:HB3  | 1:B:320:ILE:CD1  | 2.52                     | 0.40              |
| 2:K:72:LEU:C     | 2:K:72:LEU:HD13  | 2.41                     | 0.40              |
| 2:K:19:GLN:HB2   | 2:K:164:ASN:CG   | 2.41                     | 0.40              |
| 1:T:315:ARG:HH22 | 1:U:436:ASN:ND2  | 2.19                     | 0.40              |
| 1:D:352:LEU:HA   | 1:D:352:LEU:HD23 | 1.74                     | 0.40              |
| 1:A:421:ILE:HG23 | 1:A:425:TYR:HD1  | 1.80                     | 0.40              |
| 1:D:439:LEU:CD2  | 2:J:72:LEU:HG    | 2.52                     | 0.40              |
| 1:V:27:VAL:CG1   | 1:V:70:LEU:HD22  | 2.51                     | 0.40              |
| 2:O:115:PRO:HG3  | 2:O:121:LEU:HG   | 2.03                     | 0.40              |
| 1:F:283:LEU:HD23 | 1:F:283:LEU:HA   | 1.88                     | 0.40              |
| 1:C:41:GLN:CA    | 1:C:41:GLN:NE2   | 2.82                     | 0.40              |
| 1:F:316:PRO:C    | 1:F:318:ASP:N    | 2.74                     | 0.40              |
| 1:S:407:ILE:HG23 | 1:S:408:SER:N    | 2.36                     | 0.40              |
| 1:V:108:MET:SD   | 1:V:244:ALA:HB3  | 2.61                     | 0.40              |
| 1:B:71:ALA:CB    | 1:B:78:PHE:HB2   | 2.52                     | 0.40              |
| 1:U:407:ILE:HG23 | 1:U:408:SER:N    | 2.36                     | 0.40              |
| 1:D:394:ARG:O    | 1:D:396:LEU:N    | 2.55                     | 0.40              |
| 1:F:270:GLY:C    | 1:F:272:ASP:H    | 2.24                     | 0.40              |
| 1:V:391:ILE:H    | 1:V:391:ILE:HG12 | 1.57                     | 0.40              |
| 1:V:83:ALA:HB1   | 1:V:262:ILE:HG21 | 2.02                     | 0.40              |
| 2:H:95:LEU:HA    | 2:H:95:LEU:HD23  | 1.93                     | 0.40              |
| 1:S:62:GLY:HA3   | 3:S:456:ATP:C8   | 2.57                     | 0.40              |
| 2:H:18:GLY:N     | 2:H:164:ASN:HD21 | 2.06                     | 0.40              |
| 2:J:46:PHE:HB3   | 2:J:95:LEU:HD23  | 2.02                     | 0.40              |
| 1:E:17:ILE:HG22  | 1:E:18:ILE:N     | 2.36                     | 0.40              |
| 1:E:17:ILE:HG23  | 3:E:454:ATP:C6   | 2.57                     | 0.40              |
| 1:D:380:ALA:O    | 1:D:383:ARG:HB3  | 2.22                     | 0.40              |
| 1:W:32:ARG:O     | 1:W:36:ARG:HG2   | 2.22                     | 0.40              |
| 1:W:6:PRO:C      | 1:W:8:GLU:N      | 2.74                     | 0.40              |
| 1:A:36:ARG:NH1   | 1:F:360:MET:HE3  | 2.36                     | 0.40              |
| 2:G:63:LYS:HE2   | 2:G:78:LEU:HA    | 2.03                     | 0.40              |
| 1:C:378:ALA:C    | 1:C:380:ALA:N    | 2.71                     | 0.40              |
| 1:E:100:ILE:CD1  | 1:E:300:THR:HG22 | 2.52                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:43:LEU:O     | 2:R:97:VAL:HA    | 2.22                     | 0.40              |
| 1:T:79:ILE:CG2   | 1:T:103:LEU:HD13 | 2.49                     | 0.40              |
| 1:V:345:LEU:HD21 | 1:V:377:ILE:CG2  | 2.51                     | 0.40              |
| 1:A:4:MET:CE     | 1:A:9:ILE:HA     | 2.51                     | 0.40              |
| 1:B:25:ARG:O     | 1:B:28:ALA:N     | 2.55                     | 0.40              |
| 2:P:54:PHE:HA    | 2:P:57:PHE:HB3   | 2.04                     | 0.40              |
| 1:T:232:ALA:C    | 1:T:234:LEU:H    | 2.24                     | 0.40              |
| 2:G:34:VAL:HG13  | 2:G:44:ALA:O     | 2.22                     | 0.40              |
| 2:Q:78:LEU:O     | 2:Q:81:ASP:HB2   | 2.22                     | 0.40              |
| 1:F:389:GLU:O    | 1:F:395:ARG:NH2  | 2.54                     | 0.40              |
| 1:F:320:ILE:O    | 1:F:320:ILE:HG13 | 2.21                     | 0.40              |
| 2:J:68:GLN:HB3   | 2:J:68:GLN:HE21  | 1.72                     | 0.40              |
| 1:A:441:ARG:HG3  | 1:A:441:ARG:HH11 | 1.87                     | 0.40              |

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

| Atom-1        | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------------|--------------------------|-------------------|
| 1:X:7:ARG:NH2 | 1:X:7:ARG:NH2[2_765] | 2.08                     | 0.12              |

## 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     | 318/444 (72%) | 244 (77%) | 57 (18%) | 17 (5%)  | 2           | 23 |
| 1   | B     | 318/444 (72%) | 241 (76%) | 58 (18%) | 19 (6%)  | 2           | 20 |
| 1   | C     | 311/444 (70%) | 234 (75%) | 60 (19%) | 17 (6%)  | 2           | 22 |
| 1   | D     | 310/444 (70%) | 235 (76%) | 56 (18%) | 19 (6%)  | 2           | 19 |
| 1   | E     | 309/444 (70%) | 238 (77%) | 51 (16%) | 20 (6%)  | 1           | 18 |
| 1   | F     | 312/444 (70%) | 240 (77%) | 54 (17%) | 18 (6%)  | 2           | 21 |

Continued on next page...



*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured   | Allowed    | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|------------|----------|-------------|----|
| 1   | S     | 309/444 (70%)   | 227 (74%)  | 57 (18%)   | 25 (8%)  | 1           | 13 |
| 1   | T     | 323/444 (73%)   | 236 (73%)  | 63 (20%)   | 24 (7%)  | 1           | 15 |
| 1   | U     | 314/444 (71%)   | 237 (76%)  | 54 (17%)   | 23 (7%)  | 1           | 15 |
| 1   | V     | 305/444 (69%)   | 228 (75%)  | 54 (18%)   | 23 (8%)  | 1           | 14 |
| 1   | W     | 304/444 (68%)   | 223 (73%)  | 57 (19%)   | 24 (8%)  | 1           | 13 |
| 1   | X     | 314/444 (71%)   | 235 (75%)  | 56 (18%)   | 23 (7%)  | 1           | 15 |
| 2   | G     | 171/174 (98%)   | 141 (82%)  | 28 (16%)   | 2 (1%)   | 16          | 60 |
| 2   | H     | 171/174 (98%)   | 139 (81%)  | 26 (15%)   | 6 (4%)   | 4           | 36 |
| 2   | I     | 171/174 (98%)   | 136 (80%)  | 30 (18%)   | 5 (3%)   | 6           | 41 |
| 2   | J     | 171/174 (98%)   | 136 (80%)  | 28 (16%)   | 7 (4%)   | 3           | 32 |
| 2   | K     | 171/174 (98%)   | 138 (81%)  | 26 (15%)   | 7 (4%)   | 3           | 32 |
| 2   | L     | 171/174 (98%)   | 137 (80%)  | 27 (16%)   | 7 (4%)   | 3           | 32 |
| 2   | M     | 171/174 (98%)   | 128 (75%)  | 34 (20%)   | 9 (5%)   | 2           | 23 |
| 2   | N     | 171/174 (98%)   | 129 (75%)  | 34 (20%)   | 8 (5%)   | 3           | 28 |
| 2   | O     | 171/174 (98%)   | 130 (76%)  | 32 (19%)   | 9 (5%)   | 2           | 23 |
| 2   | P     | 171/174 (98%)   | 128 (75%)  | 34 (20%)   | 9 (5%)   | 2           | 23 |
| 2   | Q     | 171/174 (98%)   | 130 (76%)  | 32 (19%)   | 9 (5%)   | 2           | 23 |
| 2   | R     | 171/174 (98%)   | 128 (75%)  | 33 (19%)   | 10 (6%)  | 2           | 21 |
| All | All   | 5799/7416 (78%) | 4418 (76%) | 1041 (18%) | 340 (6%) | 2           | 21 |

All (340) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 52  | ASN  |
| 1   | A     | 235 | ILE  |
| 1   | A     | 417 | GLN  |
| 1   | A     | 436 | ASN  |
| 1   | A     | 438 | ASP  |
| 1   | A     | 441 | ARG  |
| 1   | B     | 52  | ASN  |
| 1   | B     | 231 | ALA  |
| 1   | B     | 417 | GLN  |
| 1   | B     | 438 | ASP  |
| 1   | B     | 440 | SER  |
| 1   | B     | 441 | ARG  |
| 1   | C     | 52  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 417 | GLN  |
| 1   | C     | 436 | ASN  |
| 1   | C     | 438 | ASP  |
| 1   | C     | 440 | SER  |
| 1   | C     | 441 | ARG  |
| 1   | D     | 52  | ASN  |
| 1   | D     | 435 | GLU  |
| 1   | D     | 440 | SER  |
| 1   | D     | 441 | ARG  |
| 1   | E     | 52  | ASN  |
| 1   | E     | 417 | GLN  |
| 1   | E     | 432 | GLU  |
| 1   | E     | 433 | VAL  |
| 1   | E     | 436 | ASN  |
| 1   | E     | 438 | ASP  |
| 1   | E     | 441 | ARG  |
| 1   | F     | 417 | GLN  |
| 1   | F     | 436 | ASN  |
| 1   | F     | 438 | ASP  |
| 1   | F     | 441 | ARG  |
| 2   | H     | 86  | ARG  |
| 2   | H     | 89  | ARG  |
| 2   | I     | 87  | ALA  |
| 2   | I     | 90  | LYS  |
| 2   | J     | 87  | ALA  |
| 2   | J     | 88  | LEU  |
| 2   | J     | 119 | GLN  |
| 2   | K     | 92  | GLU  |
| 2   | L     | 87  | ALA  |
| 2   | L     | 90  | LYS  |
| 2   | M     | 119 | GLN  |
| 2   | N     | 50  | THR  |
| 2   | N     | 71  | LEU  |
| 2   | P     | 71  | LEU  |
| 2   | Q     | 50  | THR  |
| 2   | Q     | 119 | GLN  |
| 2   | R     | 71  | LEU  |
| 1   | S     | 21  | ALA  |
| 1   | S     | 41  | GLN  |
| 1   | S     | 48  | VAL  |
| 1   | S     | 58  | PRO  |
| 1   | S     | 74  | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 75  | ASN  |
| 1   | S     | 235 | ILE  |
| 1   | S     | 436 | ASN  |
| 1   | S     | 437 | GLU  |
| 1   | S     | 438 | ASP  |
| 1   | S     | 440 | SER  |
| 1   | T     | 21  | ALA  |
| 1   | T     | 41  | GLN  |
| 1   | T     | 58  | PRO  |
| 1   | T     | 74  | ALA  |
| 1   | T     | 75  | ASN  |
| 1   | T     | 235 | ILE  |
| 1   | T     | 436 | ASN  |
| 1   | T     | 440 | SER  |
| 1   | T     | 442 | PHE  |
| 1   | U     | 21  | ALA  |
| 1   | U     | 41  | GLN  |
| 1   | U     | 58  | PRO  |
| 1   | U     | 74  | ALA  |
| 1   | U     | 75  | ASN  |
| 1   | U     | 235 | ILE  |
| 1   | U     | 242 | GLN  |
| 1   | U     | 442 | PHE  |
| 1   | V     | 21  | ALA  |
| 1   | V     | 41  | GLN  |
| 1   | V     | 58  | PRO  |
| 1   | V     | 74  | ALA  |
| 1   | V     | 75  | ASN  |
| 1   | V     | 440 | SER  |
| 1   | V     | 442 | PHE  |
| 1   | W     | 21  | ALA  |
| 1   | W     | 41  | GLN  |
| 1   | W     | 58  | PRO  |
| 1   | W     | 74  | ALA  |
| 1   | W     | 75  | ASN  |
| 1   | W     | 442 | PHE  |
| 1   | X     | 21  | ALA  |
| 1   | X     | 58  | PRO  |
| 1   | X     | 74  | ALA  |
| 1   | X     | 75  | ASN  |
| 1   | X     | 236 | ASN  |
| 1   | X     | 237 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 435 | GLU  |
| 1   | A     | 113 | GLN  |
| 1   | A     | 276 | GLU  |
| 1   | A     | 405 | ASP  |
| 1   | A     | 415 | ASN  |
| 1   | A     | 429 | ALA  |
| 1   | B     | 237 | PRO  |
| 1   | B     | 405 | ASP  |
| 1   | B     | 429 | ALA  |
| 1   | C     | 405 | ASP  |
| 1   | D     | 276 | GLU  |
| 1   | D     | 405 | ASP  |
| 1   | D     | 429 | ALA  |
| 1   | D     | 438 | ASP  |
| 1   | E     | 113 | GLN  |
| 1   | E     | 405 | ASP  |
| 1   | E     | 429 | ALA  |
| 1   | E     | 437 | GLU  |
| 1   | F     | 52  | ASN  |
| 1   | F     | 276 | GLU  |
| 1   | F     | 405 | ASP  |
| 1   | F     | 429 | ALA  |
| 1   | F     | 439 | LEU  |
| 1   | F     | 440 | SER  |
| 2   | J     | 89  | ARG  |
| 2   | K     | 86  | ARG  |
| 2   | L     | 86  | ARG  |
| 2   | M     | 17  | ASP  |
| 2   | M     | 50  | THR  |
| 2   | M     | 71  | LEU  |
| 2   | M     | 127 | GLY  |
| 2   | M     | 128 | ASN  |
| 2   | N     | 17  | ASP  |
| 2   | N     | 72  | LEU  |
| 2   | N     | 127 | GLY  |
| 2   | N     | 128 | ASN  |
| 2   | O     | 17  | ASP  |
| 2   | O     | 50  | THR  |
| 2   | O     | 71  | LEU  |
| 2   | O     | 72  | LEU  |
| 2   | O     | 127 | GLY  |
| 2   | O     | 128 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 17  | ASP  |
| 2   | P     | 50  | THR  |
| 2   | P     | 72  | LEU  |
| 2   | P     | 127 | GLY  |
| 2   | P     | 128 | ASN  |
| 2   | Q     | 17  | ASP  |
| 2   | Q     | 71  | LEU  |
| 2   | Q     | 72  | LEU  |
| 2   | Q     | 127 | GLY  |
| 2   | Q     | 128 | ASN  |
| 2   | R     | 17  | ASP  |
| 2   | R     | 50  | THR  |
| 2   | R     | 72  | LEU  |
| 2   | R     | 127 | GLY  |
| 2   | R     | 128 | ASN  |
| 1   | S     | 301 | ASP  |
| 1   | T     | 48  | VAL  |
| 1   | T     | 301 | ASP  |
| 1   | U     | 48  | VAL  |
| 1   | U     | 301 | ASP  |
| 1   | U     | 440 | SER  |
| 1   | V     | 48  | VAL  |
| 1   | V     | 301 | ASP  |
| 1   | W     | 48  | VAL  |
| 1   | W     | 119 | ASN  |
| 1   | W     | 301 | ASP  |
| 1   | W     | 439 | LEU  |
| 1   | X     | 41  | GLN  |
| 1   | X     | 48  | VAL  |
| 1   | X     | 301 | ASP  |
| 1   | X     | 440 | SER  |
| 1   | A     | 112 | ARG  |
| 1   | A     | 317 | SER  |
| 1   | B     | 42  | GLU  |
| 1   | B     | 294 | LYS  |
| 1   | B     | 350 | ALA  |
| 1   | B     | 411 | ALA  |
| 1   | C     | 390 | ASN  |
| 1   | C     | 429 | ALA  |
| 1   | D     | 42  | GLU  |
| 1   | D     | 240 | LEU  |
| 1   | D     | 317 | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 417 | GLN  |
| 1   | E     | 276 | GLU  |
| 1   | E     | 390 | ASN  |
| 1   | E     | 411 | ALA  |
| 1   | F     | 415 | ASN  |
| 2   | H     | 17  | ASP  |
| 2   | H     | 119 | GLN  |
| 2   | J     | 50  | THR  |
| 2   | K     | 81  | ASP  |
| 2   | K     | 89  | ARG  |
| 2   | M     | 72  | LEU  |
| 2   | M     | 117 | GLU  |
| 2   | N     | 117 | GLU  |
| 2   | O     | 117 | GLU  |
| 2   | P     | 117 | GLU  |
| 2   | R     | 117 | GLU  |
| 1   | S     | 43  | PRO  |
| 1   | S     | 44  | LEU  |
| 1   | S     | 258 | GLU  |
| 1   | S     | 439 | LEU  |
| 1   | T     | 14  | ASP  |
| 1   | T     | 43  | PRO  |
| 1   | T     | 44  | LEU  |
| 1   | T     | 233 | LYS  |
| 1   | T     | 258 | GLU  |
| 1   | T     | 394 | ARG  |
| 1   | U     | 43  | PRO  |
| 1   | U     | 44  | LEU  |
| 1   | U     | 258 | GLU  |
| 1   | V     | 43  | PRO  |
| 1   | V     | 44  | LEU  |
| 1   | V     | 435 | GLU  |
| 1   | V     | 439 | LEU  |
| 1   | W     | 43  | PRO  |
| 1   | W     | 44  | LEU  |
| 1   | W     | 258 | GLU  |
| 1   | W     | 440 | SER  |
| 1   | X     | 43  | PRO  |
| 1   | X     | 258 | GLU  |
| 1   | A     | 42  | GLU  |
| 1   | B     | 324 | GLN  |
| 1   | B     | 415 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 113 | GLN  |
| 1   | D     | 415 | ASN  |
| 1   | E     | 237 | PRO  |
| 1   | E     | 294 | LYS  |
| 1   | E     | 317 | SER  |
| 1   | F     | 4   | MET  |
| 1   | F     | 42  | GLU  |
| 1   | F     | 240 | LEU  |
| 2   | G     | 92  | GLU  |
| 2   | H     | 50  | THR  |
| 2   | I     | 17  | ASP  |
| 2   | I     | 89  | ARG  |
| 2   | J     | 91  | LEU  |
| 2   | K     | 50  | THR  |
| 2   | K     | 116 | GLU  |
| 2   | L     | 17  | ASP  |
| 2   | Q     | 117 | GLU  |
| 1   | S     | 14  | ASP  |
| 1   | S     | 20  | GLN  |
| 1   | S     | 261 | LYS  |
| 1   | S     | 313 | VAL  |
| 1   | S     | 394 | ARG  |
| 1   | T     | 20  | GLN  |
| 1   | T     | 313 | VAL  |
| 1   | T     | 438 | ASP  |
| 1   | U     | 14  | ASP  |
| 1   | U     | 20  | GLN  |
| 1   | U     | 23  | ALA  |
| 1   | U     | 313 | VAL  |
| 1   | U     | 394 | ARG  |
| 1   | V     | 14  | ASP  |
| 1   | V     | 20  | GLN  |
| 1   | V     | 23  | ALA  |
| 1   | V     | 258 | GLU  |
| 1   | W     | 14  | ASP  |
| 1   | W     | 20  | GLN  |
| 1   | W     | 313 | VAL  |
| 1   | W     | 394 | ARG  |
| 1   | X     | 14  | ASP  |
| 1   | X     | 20  | GLN  |
| 1   | X     | 23  | ALA  |
| 1   | X     | 44  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 313 | VAL  |
| 1   | X     | 394 | ARG  |
| 1   | A     | 6   | PRO  |
| 1   | B     | 317 | SER  |
| 1   | B     | 390 | ASN  |
| 1   | C     | 42  | GLU  |
| 1   | C     | 276 | GLU  |
| 1   | C     | 350 | ALA  |
| 1   | D     | 294 | LYS  |
| 1   | D     | 324 | GLN  |
| 1   | E     | 42  | GLU  |
| 1   | F     | 236 | ASN  |
| 1   | F     | 404 | MET  |
| 2   | H     | 71  | LEU  |
| 2   | I     | 50  | THR  |
| 2   | J     | 17  | ASP  |
| 2   | K     | 17  | ASP  |
| 2   | L     | 52  | ASP  |
| 1   | S     | 23  | ALA  |
| 1   | S     | 29  | ILE  |
| 1   | S     | 388 | THR  |
| 1   | T     | 23  | ALA  |
| 1   | T     | 388 | THR  |
| 1   | V     | 313 | VAL  |
| 1   | W     | 23  | ALA  |
| 1   | W     | 29  | ILE  |
| 1   | W     | 242 | GLN  |
| 1   | W     | 388 | THR  |
| 1   | A     | 440 | SER  |
| 1   | C     | 109 | LYS  |
| 1   | C     | 236 | ASN  |
| 1   | D     | 439 | LEU  |
| 1   | E     | 404 | MET  |
| 2   | G     | 9   | ASN  |
| 2   | L     | 9   | ASN  |
| 2   | L     | 50  | THR  |
| 2   | N     | 90  | LYS  |
| 2   | O     | 39  | ASN  |
| 2   | P     | 115 | PRO  |
| 2   | R     | 90  | LYS  |
| 1   | T     | 29  | ILE  |
| 1   | U     | 237 | PRO  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | U     | 388 | THR  |
| 1   | V     | 237 | PRO  |
| 1   | V     | 261 | LYS  |
| 1   | W     | 261 | LYS  |
| 1   | X     | 29  | ILE  |
| 1   | X     | 261 | LYS  |
| 1   | X     | 388 | THR  |
| 1   | B     | 6   | PRO  |
| 1   | D     | 262 | ILE  |
| 1   | E     | 6   | PRO  |
| 1   | F     | 262 | ILE  |
| 2   | Q     | 115 | PRO  |
| 1   | S     | 79  | ILE  |
| 1   | T     | 79  | ILE  |
| 1   | U     | 29  | ILE  |
| 1   | U     | 79  | ILE  |
| 1   | V     | 29  | ILE  |
| 1   | W     | 79  | ILE  |
| 1   | X     | 79  | ILE  |
| 1   | B     | 50  | PRO  |
| 1   | D     | 6   | PRO  |
| 2   | M     | 115 | PRO  |
| 2   | O     | 138 | VAL  |
| 2   | P     | 138 | VAL  |
| 1   | V     | 79  | ILE  |
| 1   | A     | 116 | ILE  |
| 1   | C     | 248 | VAL  |
| 2   | R     | 115 | PRO  |
| 1   | C     | 6   | PRO  |
| 1   | C     | 237 | PRO  |
| 1   | F     | 284 | PRO  |
| 1   | V     | 443 | ILE  |
| 2   | R     | 138 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 274/373 (74%)   | 244 (89%)  | 30 (11%) | 8           | 36 |
| 1   | B     | 274/373 (74%)   | 248 (90%)  | 26 (10%) | 11          | 43 |
| 1   | C     | 268/373 (72%)   | 231 (86%)  | 37 (14%) | 4           | 24 |
| 1   | D     | 267/373 (72%)   | 237 (89%)  | 30 (11%) | 7           | 33 |
| 1   | E     | 264/373 (71%)   | 232 (88%)  | 32 (12%) | 6           | 29 |
| 1   | F     | 269/373 (72%)   | 242 (90%)  | 27 (10%) | 9           | 40 |
| 1   | S     | 267/373 (72%)   | 246 (92%)  | 21 (8%)  | 15          | 52 |
| 1   | T     | 276/373 (74%)   | 258 (94%)  | 18 (6%)  | 21          | 62 |
| 1   | U     | 270/373 (72%)   | 250 (93%)  | 20 (7%)  | 17          | 56 |
| 1   | V     | 263/373 (70%)   | 246 (94%)  | 17 (6%)  | 21          | 62 |
| 1   | W     | 262/373 (70%)   | 246 (94%)  | 16 (6%)  | 23          | 63 |
| 1   | X     | 270/373 (72%)   | 252 (93%)  | 18 (7%)  | 20          | 61 |
| 2   | G     | 130/140 (93%)   | 115 (88%)  | 15 (12%) | 7           | 32 |
| 2   | H     | 130/140 (93%)   | 115 (88%)  | 15 (12%) | 7           | 32 |
| 2   | I     | 133/140 (95%)   | 119 (90%)  | 14 (10%) | 8           | 38 |
| 2   | J     | 130/140 (93%)   | 118 (91%)  | 12 (9%)  | 11          | 44 |
| 2   | K     | 130/140 (93%)   | 118 (91%)  | 12 (9%)  | 11          | 44 |
| 2   | L     | 133/140 (95%)   | 123 (92%)  | 10 (8%)  | 17          | 55 |
| 2   | M     | 125/140 (89%)   | 121 (97%)  | 4 (3%)   | 46          | 80 |
| 2   | N     | 125/140 (89%)   | 119 (95%)  | 6 (5%)   | 31          | 71 |
| 2   | O     | 124/140 (89%)   | 120 (97%)  | 4 (3%)   | 46          | 80 |
| 2   | P     | 124/140 (89%)   | 119 (96%)  | 5 (4%)   | 38          | 75 |
| 2   | Q     | 125/140 (89%)   | 121 (97%)  | 4 (3%)   | 46          | 80 |
| 2   | R     | 124/140 (89%)   | 119 (96%)  | 5 (4%)   | 38          | 75 |
| All | All   | 4757/6156 (77%) | 4359 (92%) | 398 (8%) | 14          | 49 |

All (398) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | THR  |
| 1   | A     | 6   | PRO  |
| 1   | A     | 20  | GLN  |
| 1   | A     | 34  | ARG  |
| 1   | A     | 39  | GLN  |
| 1   | A     | 46  | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 96  | VAL  |
| 1   | A     | 105 | ASP  |
| 1   | A     | 114 | GLN  |
| 1   | A     | 233 | LYS  |
| 1   | A     | 234 | LEU  |
| 1   | A     | 251 | ASN  |
| 1   | A     | 264 | LYS  |
| 1   | A     | 301 | ASP  |
| 1   | A     | 313 | VAL  |
| 1   | A     | 326 | ARG  |
| 1   | A     | 336 | LEU  |
| 1   | A     | 344 | ILE  |
| 1   | A     | 345 | LEU  |
| 1   | A     | 362 | THR  |
| 1   | A     | 370 | THR  |
| 1   | A     | 371 | THR  |
| 1   | A     | 379 | GLU  |
| 1   | A     | 382 | PHE  |
| 1   | A     | 384 | VAL  |
| 1   | A     | 403 | LEU  |
| 1   | A     | 410 | SER  |
| 1   | A     | 425 | TYR  |
| 1   | A     | 428 | ASP  |
| 1   | A     | 444 | LEU  |
| 1   | B     | 5   | THR  |
| 1   | B     | 20  | GLN  |
| 1   | B     | 37  | ARG  |
| 1   | B     | 39  | GLN  |
| 1   | B     | 46  | HIS  |
| 1   | B     | 82  | GLU  |
| 1   | B     | 96  | VAL  |
| 1   | B     | 105 | ASP  |
| 1   | B     | 120 | ARG  |
| 1   | B     | 251 | ASN  |
| 1   | B     | 263 | CYS  |
| 1   | B     | 264 | LYS  |
| 1   | B     | 301 | ASP  |
| 1   | B     | 313 | VAL  |
| 1   | B     | 326 | ARG  |
| 1   | B     | 336 | LEU  |
| 1   | B     | 344 | ILE  |
| 1   | B     | 345 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 362 | THR  |
| 1   | B     | 370 | THR  |
| 1   | B     | 379 | GLU  |
| 1   | B     | 382 | PHE  |
| 1   | B     | 384 | VAL  |
| 1   | B     | 403 | LEU  |
| 1   | B     | 421 | ILE  |
| 1   | B     | 440 | SER  |
| 1   | C     | 5   | THR  |
| 1   | C     | 6   | PRO  |
| 1   | C     | 20  | GLN  |
| 1   | C     | 34  | ARG  |
| 1   | C     | 39  | GLN  |
| 1   | C     | 46  | HIS  |
| 1   | C     | 82  | GLU  |
| 1   | C     | 96  | VAL  |
| 1   | C     | 105 | ASP  |
| 1   | C     | 111 | VAL  |
| 1   | C     | 118 | LYS  |
| 1   | C     | 119 | ASN  |
| 1   | C     | 251 | ASN  |
| 1   | C     | 263 | CYS  |
| 1   | C     | 264 | LYS  |
| 1   | C     | 301 | ASP  |
| 1   | C     | 308 | SER  |
| 1   | C     | 312 | GLN  |
| 1   | C     | 313 | VAL  |
| 1   | C     | 326 | ARG  |
| 1   | C     | 336 | LEU  |
| 1   | C     | 337 | SER  |
| 1   | C     | 344 | ILE  |
| 1   | C     | 345 | LEU  |
| 1   | C     | 359 | LEU  |
| 1   | C     | 362 | THR  |
| 1   | C     | 370 | THR  |
| 1   | C     | 379 | GLU  |
| 1   | C     | 382 | PHE  |
| 1   | C     | 384 | VAL  |
| 1   | C     | 403 | LEU  |
| 1   | C     | 408 | SER  |
| 1   | C     | 425 | TYR  |
| 1   | C     | 428 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 432 | GLU  |
| 1   | C     | 434 | VAL  |
| 1   | C     | 441 | ARG  |
| 1   | D     | 5   | THR  |
| 1   | D     | 6   | PRO  |
| 1   | D     | 20  | GLN  |
| 1   | D     | 25  | ARG  |
| 1   | D     | 39  | GLN  |
| 1   | D     | 46  | HIS  |
| 1   | D     | 82  | GLU  |
| 1   | D     | 96  | VAL  |
| 1   | D     | 105 | ASP  |
| 1   | D     | 108 | MET  |
| 1   | D     | 110 | LEU  |
| 1   | D     | 251 | ASN  |
| 1   | D     | 264 | LYS  |
| 1   | D     | 301 | ASP  |
| 1   | D     | 313 | VAL  |
| 1   | D     | 326 | ARG  |
| 1   | D     | 336 | LEU  |
| 1   | D     | 337 | SER  |
| 1   | D     | 344 | ILE  |
| 1   | D     | 345 | LEU  |
| 1   | D     | 362 | THR  |
| 1   | D     | 379 | GLU  |
| 1   | D     | 382 | PHE  |
| 1   | D     | 384 | VAL  |
| 1   | D     | 403 | LEU  |
| 1   | D     | 410 | SER  |
| 1   | D     | 421 | ILE  |
| 1   | D     | 428 | ASP  |
| 1   | D     | 432 | GLU  |
| 1   | D     | 434 | VAL  |
| 1   | E     | 5   | THR  |
| 1   | E     | 6   | PRO  |
| 1   | E     | 20  | GLN  |
| 1   | E     | 34  | ARG  |
| 1   | E     | 39  | GLN  |
| 1   | E     | 46  | HIS  |
| 1   | E     | 82  | GLU  |
| 1   | E     | 96  | VAL  |
| 1   | E     | 105 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 251 | ASN  |
| 1   | E     | 263 | CYS  |
| 1   | E     | 264 | LYS  |
| 1   | E     | 301 | ASP  |
| 1   | E     | 313 | VAL  |
| 1   | E     | 326 | ARG  |
| 1   | E     | 336 | LEU  |
| 1   | E     | 337 | SER  |
| 1   | E     | 344 | ILE  |
| 1   | E     | 345 | LEU  |
| 1   | E     | 362 | THR  |
| 1   | E     | 379 | GLU  |
| 1   | E     | 382 | PHE  |
| 1   | E     | 384 | VAL  |
| 1   | E     | 398 | THR  |
| 1   | E     | 402 | ARG  |
| 1   | E     | 403 | LEU  |
| 1   | E     | 408 | SER  |
| 1   | E     | 425 | TYR  |
| 1   | E     | 428 | ASP  |
| 1   | E     | 434 | VAL  |
| 1   | E     | 435 | GLU  |
| 1   | E     | 441 | ARG  |
| 1   | F     | 5   | THR  |
| 1   | F     | 20  | GLN  |
| 1   | F     | 34  | ARG  |
| 1   | F     | 39  | GLN  |
| 1   | F     | 46  | HIS  |
| 1   | F     | 82  | GLU  |
| 1   | F     | 96  | VAL  |
| 1   | F     | 105 | ASP  |
| 1   | F     | 251 | ASN  |
| 1   | F     | 264 | LYS  |
| 1   | F     | 291 | VAL  |
| 1   | F     | 301 | ASP  |
| 1   | F     | 313 | VAL  |
| 1   | F     | 321 | PRO  |
| 1   | F     | 326 | ARG  |
| 1   | F     | 336 | LEU  |
| 1   | F     | 344 | ILE  |
| 1   | F     | 345 | LEU  |
| 1   | F     | 362 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 370 | THR  |
| 1   | F     | 379 | GLU  |
| 1   | F     | 382 | PHE  |
| 1   | F     | 384 | VAL  |
| 1   | F     | 403 | LEU  |
| 1   | F     | 428 | ASP  |
| 1   | F     | 437 | GLU  |
| 1   | F     | 441 | ARG  |
| 2   | G     | 52  | ASP  |
| 2   | G     | 55  | THR  |
| 2   | G     | 56  | LEU  |
| 2   | G     | 68  | GLN  |
| 2   | G     | 72  | LEU  |
| 2   | G     | 81  | ASP  |
| 2   | G     | 82  | TRP  |
| 2   | G     | 83  | ARG  |
| 2   | G     | 84  | THR  |
| 2   | G     | 85  | ASP  |
| 2   | G     | 104 | LEU  |
| 2   | G     | 135 | ARG  |
| 2   | G     | 141 | THR  |
| 2   | G     | 164 | ASN  |
| 2   | G     | 168 | THR  |
| 2   | H     | 52  | ASP  |
| 2   | H     | 55  | THR  |
| 2   | H     | 56  | LEU  |
| 2   | H     | 68  | GLN  |
| 2   | H     | 72  | LEU  |
| 2   | H     | 82  | TRP  |
| 2   | H     | 84  | THR  |
| 2   | H     | 85  | ASP  |
| 2   | H     | 88  | LEU  |
| 2   | H     | 91  | LEU  |
| 2   | H     | 104 | LEU  |
| 2   | H     | 135 | ARG  |
| 2   | H     | 141 | THR  |
| 2   | H     | 164 | ASN  |
| 2   | H     | 168 | THR  |
| 2   | I     | 55  | THR  |
| 2   | I     | 56  | LEU  |
| 2   | I     | 68  | GLN  |
| 2   | I     | 72  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 82  | TRP  |
| 2   | I     | 85  | ASP  |
| 2   | I     | 86  | ARG  |
| 2   | I     | 88  | LEU  |
| 2   | I     | 104 | LEU  |
| 2   | I     | 119 | GLN  |
| 2   | I     | 135 | ARG  |
| 2   | I     | 141 | THR  |
| 2   | I     | 164 | ASN  |
| 2   | I     | 168 | THR  |
| 2   | J     | 52  | ASP  |
| 2   | J     | 55  | THR  |
| 2   | J     | 56  | LEU  |
| 2   | J     | 68  | GLN  |
| 2   | J     | 72  | LEU  |
| 2   | J     | 82  | TRP  |
| 2   | J     | 85  | ASP  |
| 2   | J     | 104 | LEU  |
| 2   | J     | 135 | ARG  |
| 2   | J     | 141 | THR  |
| 2   | J     | 164 | ASN  |
| 2   | J     | 168 | THR  |
| 2   | K     | 55  | THR  |
| 2   | K     | 56  | LEU  |
| 2   | K     | 68  | GLN  |
| 2   | K     | 72  | LEU  |
| 2   | K     | 82  | TRP  |
| 2   | K     | 85  | ASP  |
| 2   | K     | 88  | LEU  |
| 2   | K     | 104 | LEU  |
| 2   | K     | 135 | ARG  |
| 2   | K     | 141 | THR  |
| 2   | K     | 164 | ASN  |
| 2   | K     | 168 | THR  |
| 2   | L     | 55  | THR  |
| 2   | L     | 56  | LEU  |
| 2   | L     | 68  | GLN  |
| 2   | L     | 72  | LEU  |
| 2   | L     | 85  | ASP  |
| 2   | L     | 91  | LEU  |
| 2   | L     | 135 | ARG  |
| 2   | L     | 141 | THR  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 164 | ASN  |
| 2   | L     | 168 | THR  |
| 2   | M     | 8   | ARG  |
| 2   | M     | 137 | LEU  |
| 2   | M     | 164 | ASN  |
| 2   | M     | 167 | PHE  |
| 2   | N     | 8   | ARG  |
| 2   | N     | 52  | ASP  |
| 2   | N     | 119 | GLN  |
| 2   | N     | 137 | LEU  |
| 2   | N     | 164 | ASN  |
| 2   | N     | 167 | PHE  |
| 2   | O     | 8   | ARG  |
| 2   | O     | 137 | LEU  |
| 2   | O     | 164 | ASN  |
| 2   | O     | 167 | PHE  |
| 2   | P     | 8   | ARG  |
| 2   | P     | 52  | ASP  |
| 2   | P     | 137 | LEU  |
| 2   | P     | 164 | ASN  |
| 2   | P     | 167 | PHE  |
| 2   | Q     | 8   | ARG  |
| 2   | Q     | 137 | LEU  |
| 2   | Q     | 164 | ASN  |
| 2   | Q     | 167 | PHE  |
| 2   | R     | 8   | ARG  |
| 2   | R     | 52  | ASP  |
| 2   | R     | 137 | LEU  |
| 2   | R     | 164 | ASN  |
| 2   | R     | 167 | PHE  |
| 1   | S     | 36  | ARG  |
| 1   | S     | 75  | ASN  |
| 1   | S     | 105 | ASP  |
| 1   | S     | 114 | GLN  |
| 1   | S     | 116 | ILE  |
| 1   | S     | 246 | ASP  |
| 1   | S     | 260 | ASP  |
| 1   | S     | 322 | GLU  |
| 1   | S     | 326 | ARG  |
| 1   | S     | 333 | LEU  |
| 1   | S     | 363 | GLU  |
| 1   | S     | 366 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 388 | THR  |
| 1   | S     | 390 | ASN  |
| 1   | S     | 391 | ILE  |
| 1   | S     | 430 | LEU  |
| 1   | S     | 436 | ASN  |
| 1   | S     | 439 | LEU  |
| 1   | S     | 441 | ARG  |
| 1   | S     | 442 | PHE  |
| 1   | S     | 444 | LEU  |
| 1   | T     | 36  | ARG  |
| 1   | T     | 75  | ASN  |
| 1   | T     | 105 | ASP  |
| 1   | T     | 120 | ARG  |
| 1   | T     | 125 | ASP  |
| 1   | T     | 246 | ASP  |
| 1   | T     | 260 | ASP  |
| 1   | T     | 322 | GLU  |
| 1   | T     | 326 | ARG  |
| 1   | T     | 333 | LEU  |
| 1   | T     | 363 | GLU  |
| 1   | T     | 366 | ASN  |
| 1   | T     | 388 | THR  |
| 1   | T     | 390 | ASN  |
| 1   | T     | 430 | LEU  |
| 1   | T     | 436 | ASN  |
| 1   | T     | 439 | LEU  |
| 1   | T     | 442 | PHE  |
| 1   | U     | 36  | ARG  |
| 1   | U     | 75  | ASN  |
| 1   | U     | 105 | ASP  |
| 1   | U     | 119 | ASN  |
| 1   | U     | 120 | ARG  |
| 1   | U     | 246 | ASP  |
| 1   | U     | 260 | ASP  |
| 1   | U     | 322 | GLU  |
| 1   | U     | 326 | ARG  |
| 1   | U     | 333 | LEU  |
| 1   | U     | 363 | GLU  |
| 1   | U     | 366 | ASN  |
| 1   | U     | 388 | THR  |
| 1   | U     | 390 | ASN  |
| 1   | U     | 391 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | U     | 430 | LEU  |
| 1   | U     | 432 | GLU  |
| 1   | U     | 438 | ASP  |
| 1   | U     | 439 | LEU  |
| 1   | U     | 442 | PHE  |
| 1   | V     | 36  | ARG  |
| 1   | V     | 75  | ASN  |
| 1   | V     | 105 | ASP  |
| 1   | V     | 119 | ASN  |
| 1   | V     | 260 | ASP  |
| 1   | V     | 322 | GLU  |
| 1   | V     | 326 | ARG  |
| 1   | V     | 333 | LEU  |
| 1   | V     | 363 | GLU  |
| 1   | V     | 366 | ASN  |
| 1   | V     | 388 | THR  |
| 1   | V     | 390 | ASN  |
| 1   | V     | 391 | ILE  |
| 1   | V     | 430 | LEU  |
| 1   | V     | 432 | GLU  |
| 1   | V     | 436 | ASN  |
| 1   | V     | 442 | PHE  |
| 1   | W     | 36  | ARG  |
| 1   | W     | 75  | ASN  |
| 1   | W     | 105 | ASP  |
| 1   | W     | 246 | ASP  |
| 1   | W     | 260 | ASP  |
| 1   | W     | 322 | GLU  |
| 1   | W     | 326 | ARG  |
| 1   | W     | 333 | LEU  |
| 1   | W     | 363 | GLU  |
| 1   | W     | 366 | ASN  |
| 1   | W     | 388 | THR  |
| 1   | W     | 390 | ASN  |
| 1   | W     | 391 | ILE  |
| 1   | W     | 430 | LEU  |
| 1   | W     | 436 | ASN  |
| 1   | W     | 442 | PHE  |
| 1   | X     | 36  | ARG  |
| 1   | X     | 75  | ASN  |
| 1   | X     | 105 | ASP  |
| 1   | X     | 114 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 119 | ASN  |
| 1   | X     | 246 | ASP  |
| 1   | X     | 260 | ASP  |
| 1   | X     | 322 | GLU  |
| 1   | X     | 326 | ARG  |
| 1   | X     | 333 | LEU  |
| 1   | X     | 363 | GLU  |
| 1   | X     | 366 | ASN  |
| 1   | X     | 388 | THR  |
| 1   | X     | 390 | ASN  |
| 1   | X     | 391 | ILE  |
| 1   | X     | 430 | LEU  |
| 1   | X     | 436 | ASN  |
| 1   | X     | 442 | PHE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 39  | GLN  |
| 1   | A     | 41  | GLN  |
| 1   | A     | 75  | ASN  |
| 1   | A     | 114 | GLN  |
| 1   | A     | 236 | ASN  |
| 1   | A     | 242 | GLN  |
| 1   | A     | 250 | GLN  |
| 1   | A     | 279 | GLN  |
| 1   | A     | 324 | GLN  |
| 1   | A     | 417 | GLN  |
| 1   | B     | 20  | GLN  |
| 1   | B     | 39  | GLN  |
| 1   | B     | 41  | GLN  |
| 1   | B     | 236 | ASN  |
| 1   | B     | 250 | GLN  |
| 1   | B     | 279 | GLN  |
| 1   | B     | 324 | GLN  |
| 1   | B     | 397 | HIS  |
| 1   | B     | 417 | GLN  |
| 1   | B     | 436 | ASN  |
| 1   | C     | 20  | GLN  |
| 1   | C     | 39  | GLN  |
| 1   | C     | 41  | GLN  |
| 1   | C     | 52  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 114 | GLN  |
| 1   | C     | 250 | GLN  |
| 1   | C     | 279 | GLN  |
| 1   | C     | 295 | HIS  |
| 1   | C     | 324 | GLN  |
| 1   | C     | 397 | HIS  |
| 1   | C     | 417 | GLN  |
| 1   | D     | 39  | GLN  |
| 1   | D     | 41  | GLN  |
| 1   | D     | 114 | GLN  |
| 1   | D     | 250 | GLN  |
| 1   | D     | 279 | GLN  |
| 1   | D     | 324 | GLN  |
| 1   | D     | 417 | GLN  |
| 1   | E     | 20  | GLN  |
| 1   | E     | 39  | GLN  |
| 1   | E     | 41  | GLN  |
| 1   | E     | 52  | ASN  |
| 1   | E     | 75  | ASN  |
| 1   | E     | 114 | GLN  |
| 1   | E     | 250 | GLN  |
| 1   | E     | 279 | GLN  |
| 1   | E     | 324 | GLN  |
| 1   | E     | 417 | GLN  |
| 1   | F     | 20  | GLN  |
| 1   | F     | 39  | GLN  |
| 1   | F     | 41  | GLN  |
| 1   | F     | 250 | GLN  |
| 1   | F     | 279 | GLN  |
| 1   | F     | 295 | HIS  |
| 1   | F     | 324 | GLN  |
| 1   | F     | 417 | GLN  |
| 2   | G     | 24  | ASN  |
| 2   | G     | 30  | ASN  |
| 2   | G     | 164 | ASN  |
| 2   | H     | 24  | ASN  |
| 2   | H     | 30  | ASN  |
| 2   | H     | 164 | ASN  |
| 2   | I     | 24  | ASN  |
| 2   | I     | 30  | ASN  |
| 2   | I     | 164 | ASN  |
| 2   | J     | 24  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 164 | ASN  |
| 2   | K     | 24  | ASN  |
| 2   | K     | 30  | ASN  |
| 2   | K     | 164 | ASN  |
| 2   | L     | 24  | ASN  |
| 2   | L     | 30  | ASN  |
| 2   | L     | 164 | ASN  |
| 2   | M     | 164 | ASN  |
| 2   | N     | 119 | GLN  |
| 2   | N     | 164 | ASN  |
| 2   | O     | 164 | ASN  |
| 2   | P     | 164 | ASN  |
| 2   | Q     | 164 | ASN  |
| 2   | R     | 164 | ASN  |
| 1   | S     | 41  | GLN  |
| 1   | S     | 75  | ASN  |
| 1   | S     | 236 | ASN  |
| 1   | S     | 279 | GLN  |
| 1   | S     | 366 | ASN  |
| 1   | S     | 385 | ASN  |
| 1   | S     | 390 | ASN  |
| 1   | S     | 436 | ASN  |
| 1   | T     | 41  | GLN  |
| 1   | T     | 75  | ASN  |
| 1   | T     | 119 | ASN  |
| 1   | T     | 279 | GLN  |
| 1   | T     | 324 | GLN  |
| 1   | T     | 366 | ASN  |
| 1   | T     | 385 | ASN  |
| 1   | T     | 390 | ASN  |
| 1   | T     | 436 | ASN  |
| 1   | U     | 41  | GLN  |
| 1   | U     | 75  | ASN  |
| 1   | U     | 119 | ASN  |
| 1   | U     | 279 | GLN  |
| 1   | U     | 324 | GLN  |
| 1   | U     | 366 | ASN  |
| 1   | U     | 385 | ASN  |
| 1   | U     | 390 | ASN  |
| 1   | U     | 436 | ASN  |
| 1   | V     | 41  | GLN  |
| 1   | V     | 75  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | V     | 119 | ASN  |
| 1   | V     | 236 | ASN  |
| 1   | V     | 279 | GLN  |
| 1   | V     | 366 | ASN  |
| 1   | V     | 385 | ASN  |
| 1   | V     | 390 | ASN  |
| 1   | V     | 397 | HIS  |
| 1   | W     | 41  | GLN  |
| 1   | W     | 75  | ASN  |
| 1   | W     | 119 | ASN  |
| 1   | W     | 279 | GLN  |
| 1   | W     | 324 | GLN  |
| 1   | W     | 366 | ASN  |
| 1   | W     | 385 | ASN  |
| 1   | W     | 390 | ASN  |
| 1   | X     | 41  | GLN  |
| 1   | X     | 75  | ASN  |
| 1   | X     | 114 | GLN  |
| 1   | X     | 119 | ASN  |
| 1   | X     | 279 | GLN  |
| 1   | X     | 366 | ASN  |
| 1   | X     | 385 | ASN  |
| 1   | X     | 390 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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 | $\# Z  > 2$ |
| 3   | ATP  | A     | 450 | -    | 24,33,33     | 0.78 | 0           | 31,52,52    | 1.11 | 2 (6%)      |
| 3   | ATP  | B     | 451 | -    | 24,33,33     | 0.72 | 0           | 31,52,52    | 1.25 | 4 (12%)     |
| 3   | ATP  | C     | 452 | -    | 24,33,33     | 0.69 | 0           | 31,52,52    | 1.54 | 5 (16%)     |
| 3   | ATP  | D     | 453 | -    | 24,33,33     | 0.67 | 0           | 31,52,52    | 1.36 | 4 (12%)     |
| 3   | ATP  | E     | 454 | -    | 24,33,33     | 0.78 | 0           | 31,52,52    | 1.37 | 3 (9%)      |
| 3   | ATP  | F     | 455 | -    | 24,33,33     | 0.76 | 0           | 31,52,52    | 1.15 | 2 (6%)      |
| 3   | ATP  | S     | 456 | -    | 24,33,33     | 0.58 | 0           | 31,52,52    | 0.90 | 1 (3%)      |
| 3   | ATP  | T     | 457 | -    | 24,33,33     | 0.63 | 0           | 31,52,52    | 0.88 | 1 (3%)      |
| 3   | ATP  | U     | 458 | -    | 24,33,33     | 0.57 | 0           | 31,52,52    | 0.89 | 1 (3%)      |
| 3   | ATP  | V     | 459 | -    | 24,33,33     | 0.58 | 0           | 31,52,52    | 0.86 | 1 (3%)      |
| 3   | ATP  | W     | 460 | -    | 24,33,33     | 0.62 | 0           | 31,52,52    | 0.91 | 1 (3%)      |
| 3   | ATP  | X     | 461 | -    | 24,33,33     | 0.59 | 0           | 31,52,52    | 0.88 | 1 (3%)      |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | ATP  | A     | 450 | -    | -       | 0/18/38/38 | 0/3/3/3 |
| 3   | ATP  | B     | 451 | -    | -       | 0/18/38/38 | 0/3/3/3 |
| 3   | ATP  | C     | 452 | -    | -       | 0/18/38/38 | 0/3/3/3 |
| 3   | ATP  | D     | 453 | -    | -       | 0/18/38/38 | 0/3/3/3 |
| 3   | ATP  | E     | 454 | -    | -       | 0/18/38/38 | 0/3/3/3 |
| 3   | ATP  | F     | 455 | -    | -       | 0/18/38/38 | 0/3/3/3 |
| 3   | ATP  | S     | 456 | -    | -       | 0/18/38/38 | 0/3/3/3 |
| 3   | ATP  | T     | 457 | -    | -       | 0/18/38/38 | 0/3/3/3 |
| 3   | ATP  | U     | 458 | -    | -       | 0/18/38/38 | 0/3/3/3 |
| 3   | ATP  | V     | 459 | -    | -       | 0/18/38/38 | 0/3/3/3 |
| 3   | ATP  | W     | 460 | -    | -       | 0/18/38/38 | 0/3/3/3 |
| 3   | ATP  | X     | 461 | -    | -       | 0/18/38/38 | 0/3/3/3 |



There are no bond length outliers.

All (26) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | E     | 454 | ATP  | C2'-C1'-N9 | -4.74 | 107.05      | 114.29   |
| 3   | C     | 452 | ATP  | PA-O3A-PB  | -4.28 | 120.71      | 132.73   |
| 3   | D     | 453 | ATP  | C2'-C1'-N9 | -3.32 | 109.23      | 114.29   |
| 3   | C     | 452 | ATP  | C2'-C1'-N9 | -2.86 | 109.92      | 114.29   |
| 3   | F     | 455 | ATP  | C2'-C1'-N9 | -2.56 | 110.38      | 114.29   |
| 3   | A     | 450 | ATP  | PA-O3A-PB  | -2.51 | 125.69      | 132.73   |
| 3   | B     | 451 | ATP  | C2'-C1'-N9 | -2.36 | 110.68      | 114.29   |
| 3   | B     | 451 | ATP  | PA-O3A-PB  | -2.28 | 126.33      | 132.73   |
| 3   | D     | 453 | ATP  | PA-O3A-PB  | -2.27 | 126.36      | 132.73   |
| 3   | A     | 450 | ATP  | O3G-PG-O2G | 2.13  | 115.50      | 107.38   |
| 3   | E     | 454 | ATP  | O3G-PG-O2G | 2.24  | 115.92      | 107.38   |
| 3   | C     | 452 | ATP  | O3G-PG-O2G | 2.25  | 115.96      | 107.38   |
| 3   | B     | 451 | ATP  | O3G-PG-O2G | 2.30  | 116.13      | 107.38   |
| 3   | V     | 459 | ATP  | O3G-PG-O2G | 2.34  | 116.29      | 107.38   |
| 3   | S     | 456 | ATP  | O3G-PG-O2G | 2.36  | 116.36      | 107.38   |
| 3   | T     | 457 | ATP  | O3G-PG-O2G | 2.36  | 116.38      | 107.38   |
| 3   | U     | 458 | ATP  | O3G-PG-O2G | 2.38  | 116.45      | 107.38   |
| 3   | X     | 461 | ATP  | O3G-PG-O2G | 2.40  | 116.51      | 107.38   |
| 3   | W     | 460 | ATP  | O3G-PG-O2G | 2.40  | 116.53      | 107.38   |
| 3   | F     | 455 | ATP  | O3G-PG-O2G | 2.41  | 116.56      | 107.38   |
| 3   | C     | 452 | ATP  | PB-O3B-PG  | 2.42  | 140.78      | 132.67   |
| 3   | D     | 453 | ATP  | PB-O3B-PG  | 2.44  | 140.86      | 132.67   |
| 3   | E     | 454 | ATP  | O3A-PA-O5' | 2.85  | 110.49      | 102.94   |
| 3   | D     | 453 | ATP  | O3A-PA-O5' | 3.03  | 110.98      | 102.94   |
| 3   | B     | 451 | ATP  | O3A-PA-O5' | 3.60  | 112.47      | 102.94   |
| 3   | C     | 452 | ATP  | O3A-PA-O5' | 4.26  | 114.25      | 102.94   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 82 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 450 | ATP  | 2       | 0            |
| 3   | B     | 451 | ATP  | 5       | 0            |
| 3   | C     | 452 | ATP  | 5       | 0            |
| 3   | D     | 453 | ATP  | 4       | 0            |
| 3   | E     | 454 | ATP  | 9       | 0            |
| 3   | F     | 455 | ATP  | 8       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | S     | 456 | ATP  | 14      | 0            |
| 3   | T     | 457 | ATP  | 3       | 0            |
| 3   | U     | 458 | ATP  | 12      | 0            |
| 3   | V     | 459 | ATP  | 3       | 0            |
| 3   | W     | 460 | ATP  | 8       | 0            |
| 3   | X     | 461 | ATP  | 9       | 0            |

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.