



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 10:49 AM UTC

PDB ID : 5KNW / pdb\_00005knw  
BMRB ID : 30126  
Title : Solution NMR structure of human LARP7 xRRM2  
Authors : Eichhorn, C.D.; Feigon, J.  
Deposited on : 2016-06-28

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

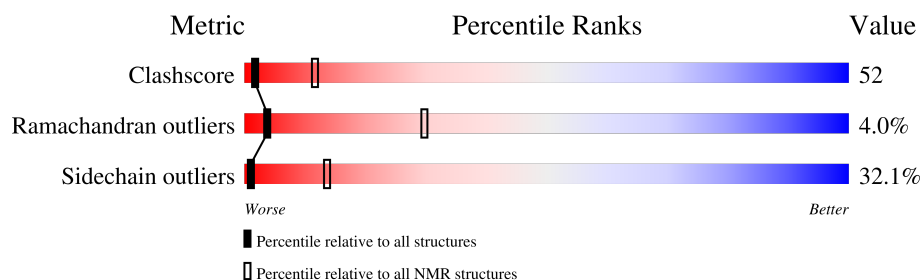
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

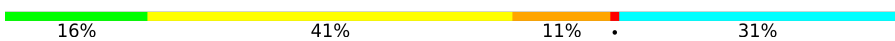
The overall completeness of chemical shifts assignment is 91%.

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) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 125    |  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:455-A:540 (86)      | 0.54              | 3            |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 2 single-model clusters were found.

| Cluster number        | Models                                   |
|-----------------------|------------------------------------------|
| 1                     | 1, 3, 4, 6, 8, 9, 10, 15, 16, 17, 19, 20 |
| 2                     | 7, 12, 14, 18                            |
| 3                     | 11, 13                                   |
| Single-model clusters | 2; 5                                     |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2042 atoms, of which 1029 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called La-related protein 7.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 125      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2042  | 636 | 1029 | 189 | 185 | 3 |       |

There are 8 discrepancies between the modelled and reference sequences:

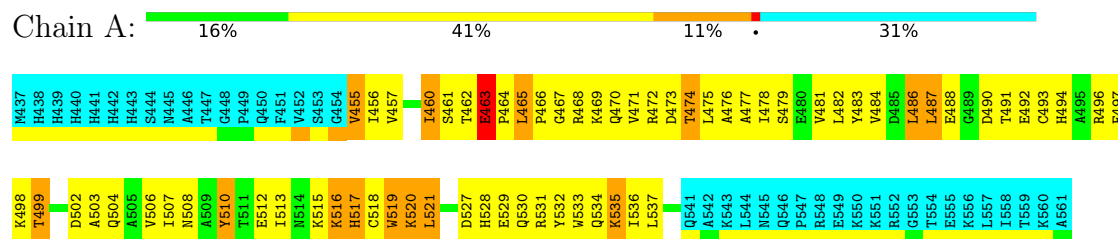
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 437     | MET      | -      | initiating methionine | UNP Q4G0J3 |
| A     | 438     | HIS      | -      | expression tag        | UNP Q4G0J3 |
| A     | 439     | HIS      | -      | expression tag        | UNP Q4G0J3 |
| A     | 440     | HIS      | -      | expression tag        | UNP Q4G0J3 |
| A     | 441     | HIS      | -      | expression tag        | UNP Q4G0J3 |
| A     | 442     | HIS      | -      | expression tag        | UNP Q4G0J3 |
| A     | 443     | HIS      | -      | expression tag        | UNP Q4G0J3 |
| A     | 444     | SER      | -      | expression tag        | UNP Q4G0J3 |

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: La-related protein 7

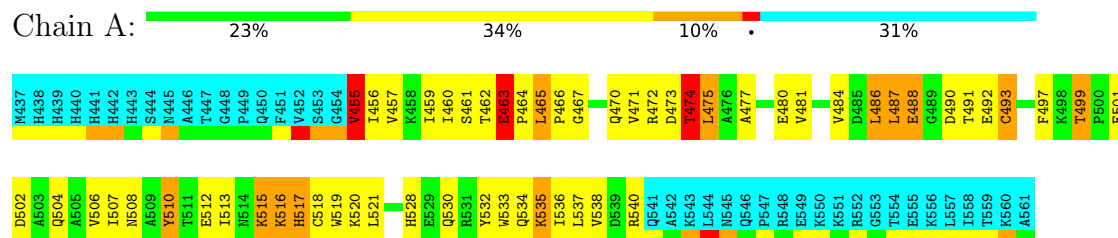


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

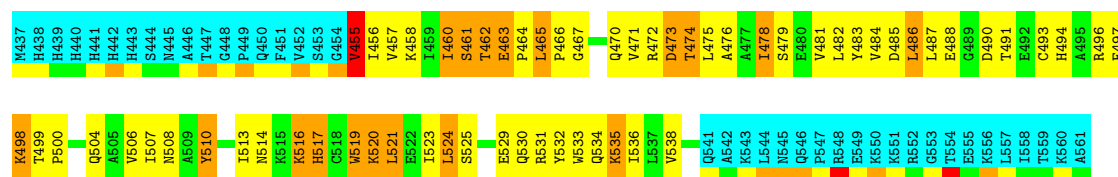
- Molecule 1: La-related protein 7



#### 4.2.2 Score per residue for model 2

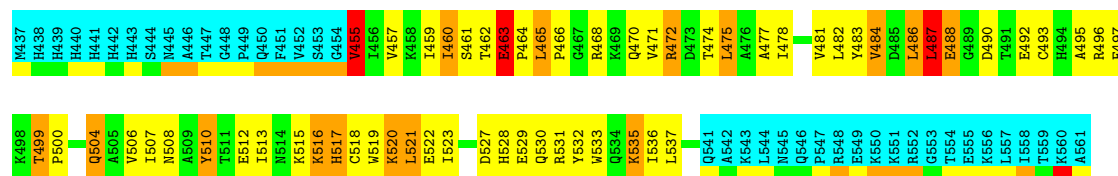
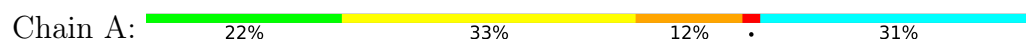
- Molecule 1: La-related protein 7





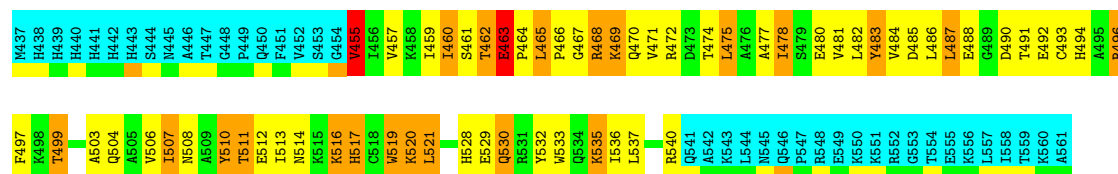
### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: La-related protein 7



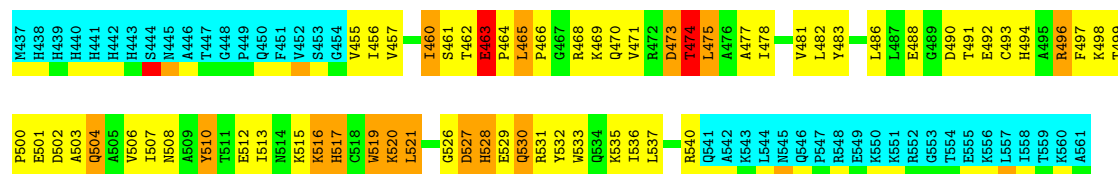
### 4.2.4 Score per residue for model 4

- Molecule 1: La-related protein 7



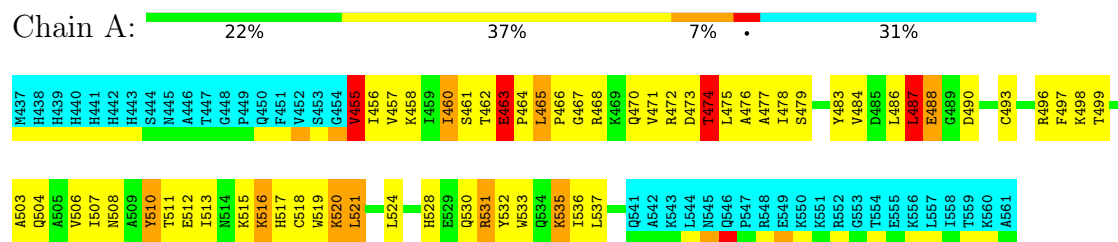
### 4.2.5 Score per residue for model 5

- Molecule 1: La-related protein 7



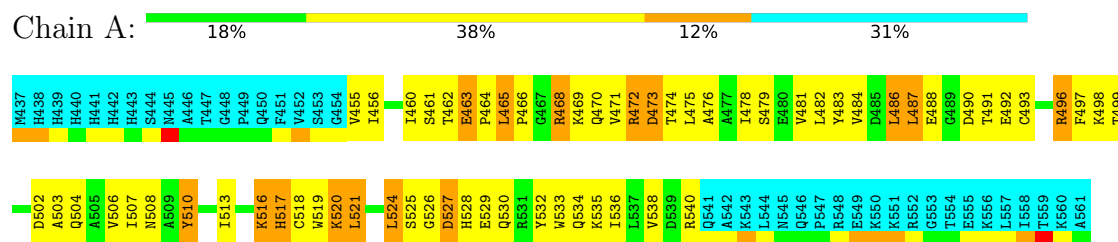
### 4.2.6 Score per residue for model 6

- Molecule 1: La-related protein 7



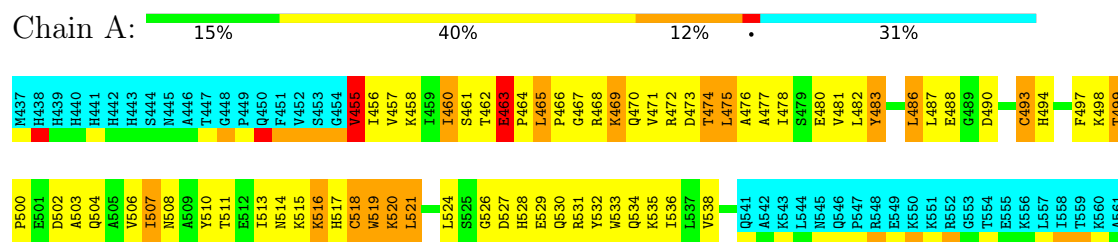
#### 4.2.7 Score per residue for model 7

- Molecule 1: La-related protein 7



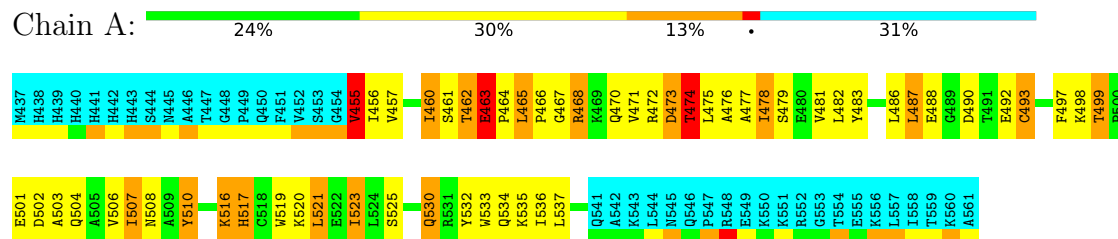
#### 4.2.8 Score per residue for model 8

- Molecule 1: La-related protein 7



#### 4.2.9 Score per residue for model 9

- Molecule 1: La-related protein 7



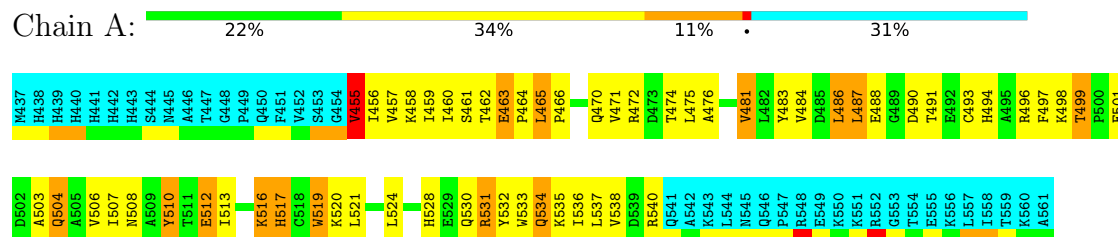
### 4.2.10 Score per residue for model 10

- Molecule 1: La-related protein 7



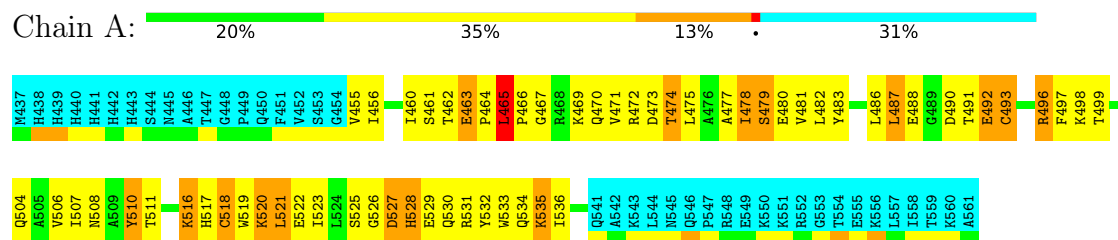
### 4.2.11 Score per residue for model 11

- Molecule 1: La-related protein 7



### 4.2.12 Score per residue for model 12

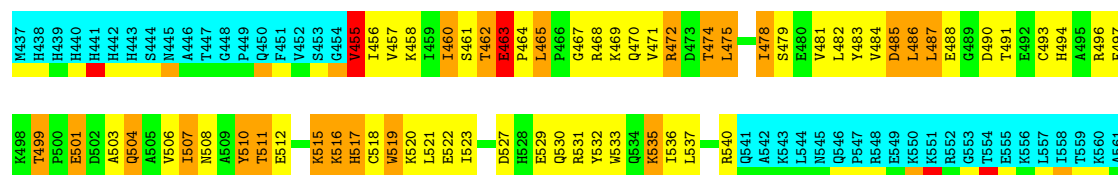
- Molecule 1: La-related protein 7



### 4.2.13 Score per residue for model 13

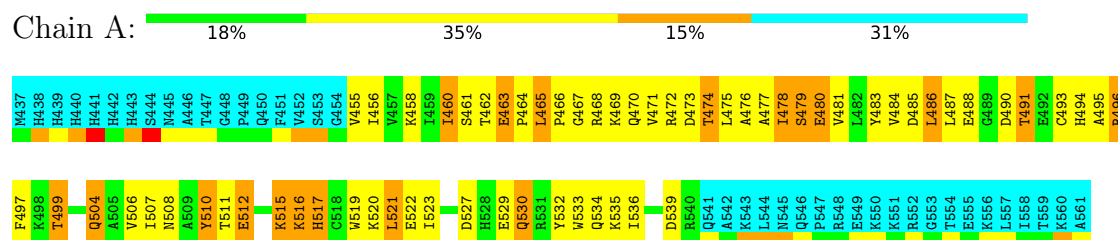
- Molecule 1: La-related protein 7





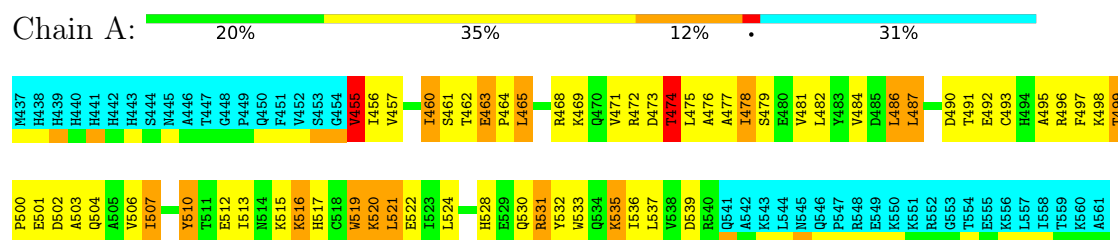
#### 4.2.14 Score per residue for model 14

- Molecule 1: La-related protein 7



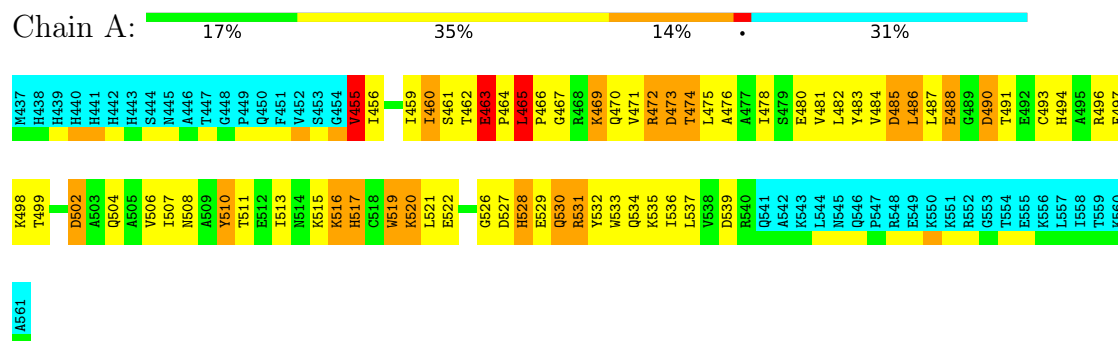
#### 4.2.15 Score per residue for model 15

- Molecule 1: La-related protein 7



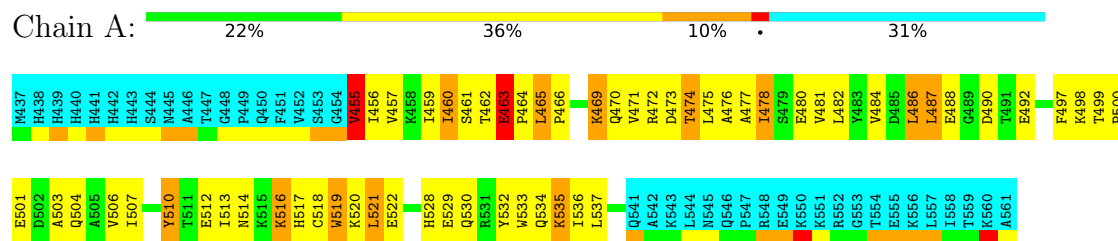
#### 4.2.16 Score per residue for model 16

- Molecule 1: La-related protein 7



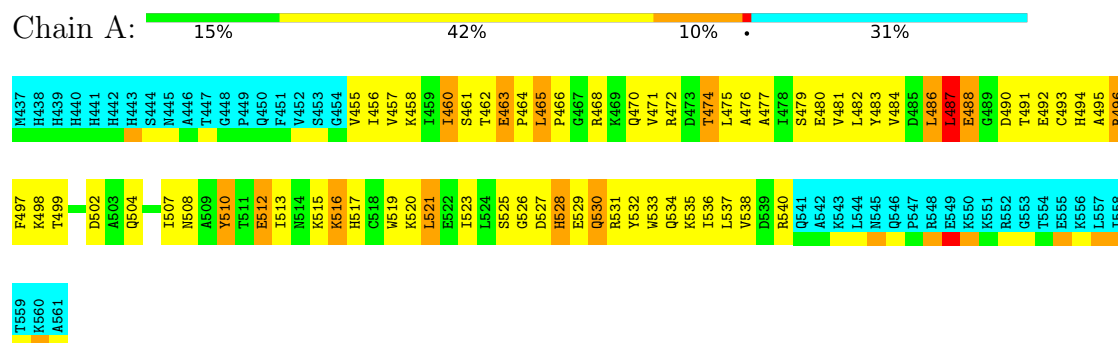
## 4.2.17 Score per residue for model 17

- Molecule 1: La-related protein 7



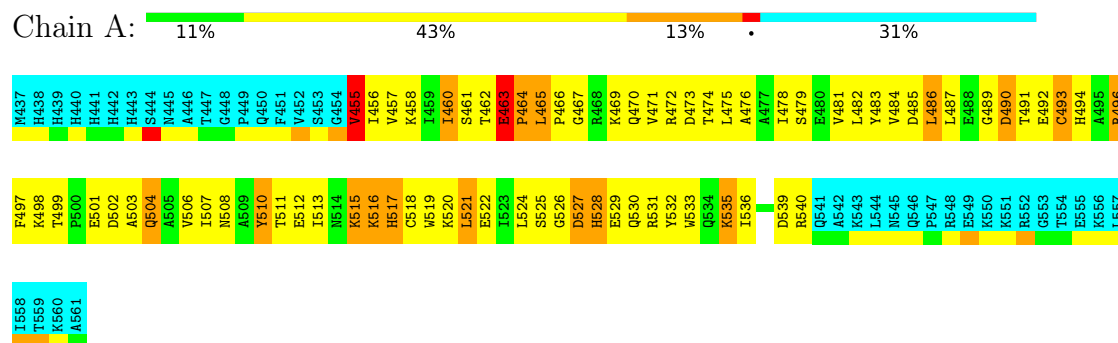
## 4.2.18 Score per residue for model 18

- Molecule 1: La-related protein 7



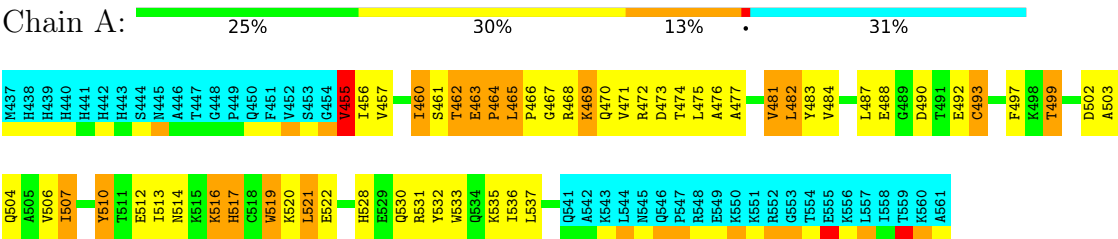
## 4.2.19 Score per residue for model 19

- Molecule 1: La-related protein 7



## 4.2.20 Score per residue for model 20

- Molecule 1: La-related protein 7



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| TALOS         | geometry optimization |         |
| CYANA         | structure calculation | 2.1     |
| X-PLOR NIH    | refinement            |         |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1514           |
| Number of shifts mapped to atoms             | 1514           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 91%            |

## 6 Model quality

### 6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 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 each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 700   | 711      | 708      | 73±9    |
| All | All   | 14000 | 14220    | 14160    | 1466    |

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 52.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:510:TYR:CD1  | 1:A:521:LEU:HD13 | 0.97     | 1.94        | 2      | 4     |
| 1:A:520:LYS:O    | 1:A:521:LEU:HD13 | 0.95     | 1.60        | 8      | 7     |
| 1:A:486:LEU:HD22 | 1:A:487:LEU:N    | 0.93     | 1.78        | 15     | 3     |
| 1:A:510:TYR:CG   | 1:A:521:LEU:HD12 | 0.92     | 2.00        | 6      | 3     |
| 1:A:486:LEU:HD12 | 1:A:487:LEU:N    | 0.92     | 1.79        | 13     | 3     |
| 1:A:510:TYR:CD1  | 1:A:521:LEU:HD22 | 0.90     | 2.00        | 13     | 6     |
| 1:A:475:LEU:CD1  | 1:A:481:VAL:HG21 | 0.90     | 1.97        | 18     | 15    |
| 1:A:467:GLY:O    | 1:A:471:VAL:HG23 | 0.88     | 1.68        | 20     | 11    |
| 1:A:520:LYS:C    | 1:A:521:LEU:HD13 | 0.87     | 1.94        | 15     | 6     |
| 1:A:507:ILE:HD12 | 1:A:508:ASN:N    | 0.87     | 1.85        | 12     | 9     |
| 1:A:510:TYR:CD1  | 1:A:521:LEU:HD12 | 0.86     | 2.05        | 6      | 3     |
| 1:A:456:ILE:HD11 | 1:A:533:TRP:CE2  | 0.86     | 2.06        | 20     | 10    |
| 1:A:507:ILE:HG22 | 1:A:521:LEU:CB   | 0.85     | 2.01        | 15     | 5     |
| 1:A:461:SER:OG   | 1:A:465:LEU:HD12 | 0.84     | 1.72        | 17     | 10    |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:507:ILE:HA   | 1:A:521:LEU:HD23 | 0.84     | 1.47        | 1      | 3     |
| 1:A:484:VAL:HG13 | 1:A:495:ALA:HB2  | 0.83     | 1.49        | 3      | 3     |
| 1:A:461:SER:HB3  | 1:A:465:LEU:HD12 | 0.82     | 1.52        | 9      | 8     |
| 1:A:460:ILE:HG22 | 1:A:520:LYS:HB2  | 0.81     | 1.52        | 14     | 20    |
| 1:A:507:ILE:HG22 | 1:A:521:LEU:HB3  | 0.81     | 1.51        | 8      | 10    |
| 1:A:486:LEU:HD12 | 1:A:493:CYS:HB3  | 0.79     | 1.55        | 3      | 4     |
| 1:A:481:VAL:HG12 | 1:A:497:PHE:CE1  | 0.78     | 2.13        | 8      | 9     |
| 1:A:510:TYR:CG   | 1:A:521:LEU:HD22 | 0.77     | 2.14        | 13     | 4     |
| 1:A:457:VAL:HG21 | 1:A:497:PHE:CE1  | 0.77     | 2.14        | 20     | 4     |
| 1:A:532:TYR:CE1  | 1:A:536:ILE:HD11 | 0.77     | 2.15        | 13     | 19    |
| 1:A:465:LEU:HD21 | 1:A:471:VAL:HG21 | 0.76     | 1.57        | 8      | 5     |
| 1:A:478:ILE:HD13 | 1:A:506:VAL:HG23 | 0.76     | 1.56        | 10     | 2     |
| 1:A:486:LEU:HD12 | 1:A:493:CYS:HB2  | 0.75     | 1.58        | 11     | 4     |
| 1:A:521:LEU:HD22 | 1:A:521:LEU:N    | 0.75     | 1.96        | 3      | 7     |
| 1:A:510:TYR:CE1  | 1:A:521:LEU:HD13 | 0.74     | 2.16        | 7      | 5     |
| 1:A:474:THR:O    | 1:A:478:ILE:HD12 | 0.74     | 1.82        | 16     | 6     |
| 1:A:457:VAL:HG21 | 1:A:497:PHE:CE2  | 0.74     | 2.18        | 15     | 10    |
| 1:A:510:TYR:CE2  | 1:A:513:ILE:HD11 | 0.74     | 2.17        | 19     | 1     |
| 1:A:481:VAL:HG12 | 1:A:497:PHE:CE2  | 0.74     | 2.18        | 14     | 5     |
| 1:A:533:TRP:CE3  | 1:A:536:ILE:HD12 | 0.73     | 2.18        | 5      | 18    |
| 1:A:455:VAL:HG11 | 1:A:500:PRO:HA   | 0.73     | 1.59        | 3      | 5     |
| 1:A:502:ASP:O    | 1:A:506:VAL:HG23 | 0.73     | 1.83        | 16     | 3     |
| 1:A:513:ILE:HG22 | 1:A:517:HIS:O    | 0.73     | 1.83        | 15     | 6     |
| 1:A:457:VAL:HG23 | 1:A:523:ILE:HD13 | 0.72     | 1.61        | 13     | 1     |
| 1:A:534:GLN:O    | 1:A:538:VAL:HG23 | 0.72     | 1.83        | 11     | 7     |
| 1:A:487:LEU:HD22 | 1:A:492:GLU:CG   | 0.71     | 2.15        | 7      | 1     |
| 1:A:465:LEU:HD13 | 1:A:491:THR:HA   | 0.71     | 1.61        | 19     | 1     |
| 1:A:507:ILE:HG22 | 1:A:521:LEU:HB2  | 0.71     | 1.62        | 15     | 1     |
| 1:A:456:ILE:HD11 | 1:A:533:TRP:CZ2  | 0.71     | 2.20        | 5      | 8     |
| 1:A:471:VAL:HG11 | 1:A:493:CYS:SG   | 0.71     | 2.26        | 13     | 5     |
| 1:A:520:LYS:C    | 1:A:521:LEU:HD22 | 0.70     | 2.12        | 18     | 5     |
| 1:A:482:LEU:C    | 1:A:482:LEU:HD12 | 0.69     | 2.12        | 20     | 1     |
| 1:A:532:TYR:HE1  | 1:A:536:ILE:HD11 | 0.69     | 1.46        | 8      | 20    |
| 1:A:468:ARG:HA   | 1:A:486:LEU:HD13 | 0.69     | 1.63        | 4      | 2     |
| 1:A:486:LEU:O    | 1:A:486:LEU:HD13 | 0.69     | 1.87        | 2      | 1     |
| 1:A:484:VAL:HG23 | 1:A:495:ALA:HB2  | 0.69     | 1.64        | 18     | 1     |
| 1:A:455:VAL:HG21 | 1:A:499:THR:C    | 0.68     | 2.13        | 4      | 12    |
| 1:A:465:LEU:HD13 | 1:A:491:THR:CA   | 0.68     | 2.18        | 19     | 3     |
| 1:A:486:LEU:HD23 | 1:A:493:CYS:HB2  | 0.68     | 1.64        | 15     | 2     |
| 1:A:465:LEU:HD21 | 1:A:493:CYS:SG   | 0.67     | 2.29        | 20     | 1     |
| 1:A:507:ILE:HG22 | 1:A:521:LEU:CG   | 0.67     | 2.19        | 14     | 4     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:478:ILE:HG22 | 1:A:506:VAL:HG22 | 0.67     | 1.67        | 2      | 1     |
| 1:A:481:VAL:HG12 | 1:A:497:PHE:CD2  | 0.66     | 2.26        | 14     | 3     |
| 1:A:482:LEU:HD12 | 1:A:498:LYS:CG   | 0.66     | 2.19        | 2      | 1     |
| 1:A:507:ILE:HA   | 1:A:521:LEU:HD21 | 0.66     | 1.66        | 14     | 2     |
| 1:A:471:VAL:HG13 | 1:A:519:TRP:CH2  | 0.66     | 2.25        | 19     | 5     |
| 1:A:486:LEU:HD12 | 1:A:486:LEU:C    | 0.66     | 2.15        | 13     | 3     |
| 1:A:486:LEU:HD12 | 1:A:493:CYS:SG   | 0.65     | 2.32        | 12     | 2     |
| 1:A:478:ILE:HD13 | 1:A:510:TYR:CE2  | 0.65     | 2.27        | 2      | 5     |
| 1:A:507:ILE:HG22 | 1:A:521:LEU:HD11 | 0.65     | 1.69        | 7      | 1     |
| 1:A:478:ILE:HD13 | 1:A:510:TYR:HE2  | 0.65     | 1.49        | 2      | 7     |
| 1:A:510:TYR:CD1  | 1:A:521:LEU:CD1  | 0.65     | 2.80        | 10     | 5     |
| 1:A:484:VAL:HG13 | 1:A:484:VAL:O    | 0.64     | 1.92        | 6      | 6     |
| 1:A:507:ILE:HG22 | 1:A:521:LEU:HD21 | 0.64     | 1.69        | 2      | 3     |
| 1:A:486:LEU:HD22 | 1:A:489:GLY:CA   | 0.64     | 2.22        | 19     | 1     |
| 1:A:461:SER:CB   | 1:A:465:LEU:HD12 | 0.64     | 2.23        | 3      | 18    |
| 1:A:460:ILE:HD13 | 1:A:461:SER:N    | 0.63     | 2.08        | 15     | 12    |
| 1:A:486:LEU:HD13 | 1:A:486:LEU:C    | 0.63     | 2.17        | 2      | 1     |
| 1:A:481:VAL:CG1  | 1:A:497:PHE:CE1  | 0.63     | 2.81        | 17     | 3     |
| 1:A:460:ILE:HD13 | 1:A:461:SER:O    | 0.63     | 1.92        | 16     | 14    |
| 1:A:536:ILE:HG23 | 1:A:540:ARG:NH1  | 0.63     | 2.09        | 18     | 1     |
| 1:A:457:VAL:HG23 | 1:A:523:ILE:CD1  | 0.63     | 2.23        | 13     | 1     |
| 1:A:457:VAL:CG2  | 1:A:497:PHE:CE1  | 0.62     | 2.82        | 20     | 3     |
| 1:A:486:LEU:HD22 | 1:A:489:GLY:HA2  | 0.62     | 1.71        | 19     | 1     |
| 1:A:507:ILE:HG22 | 1:A:521:LEU:HG   | 0.62     | 1.70        | 14     | 3     |
| 1:A:457:VAL:CG2  | 1:A:497:PHE:CE2  | 0.62     | 2.81        | 15     | 9     |
| 1:A:468:ARG:HD3  | 1:A:486:LEU:HD22 | 0.62     | 1.72        | 9      | 1     |
| 1:A:472:ARG:HB3  | 1:A:484:VAL:HG11 | 0.61     | 1.73        | 20     | 3     |
| 1:A:457:VAL:HG21 | 1:A:497:PHE:CZ   | 0.61     | 2.31        | 15     | 2     |
| 1:A:507:ILE:CB   | 1:A:521:LEU:HD21 | 0.61     | 2.26        | 2      | 2     |
| 1:A:465:LEU:CD2  | 1:A:471:VAL:HG21 | 0.60     | 2.26        | 5      | 6     |
| 1:A:481:VAL:CG1  | 1:A:497:PHE:CE2  | 0.60     | 2.84        | 14     | 2     |
| 1:A:521:LEU:HD23 | 1:A:521:LEU:O    | 0.60     | 1.95        | 7      | 3     |
| 1:A:486:LEU:HD13 | 1:A:493:CYS:HB3  | 0.60     | 1.70        | 10     | 2     |
| 1:A:479:SER:HB3  | 1:A:506:VAL:HG22 | 0.60     | 1.72        | 12     | 2     |
| 1:A:471:VAL:HG22 | 1:A:519:TRP:CZ2  | 0.59     | 2.32        | 15     | 9     |
| 1:A:532:TYR:CE2  | 1:A:535:LYS:CE   | 0.59     | 2.85        | 16     | 3     |
| 1:A:510:TYR:CD2  | 1:A:513:ILE:HD11 | 0.59     | 2.32        | 19     | 1     |
| 1:A:468:ARG:HB3  | 1:A:486:LEU:HD23 | 0.59     | 1.74        | 18     | 2     |
| 1:A:475:LEU:HD12 | 1:A:481:VAL:HG21 | 0.59     | 1.72        | 11     | 5     |
| 1:A:507:ILE:HG22 | 1:A:521:LEU:CD2  | 0.59     | 2.27        | 14     | 2     |
| 1:A:457:VAL:CG1  | 1:A:521:LEU:CD2  | 0.59     | 2.81        | 6      | 3     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:533:TRP:O    | 1:A:537:LEU:HD12 | 0.59     | 1.98        | 4      | 1     |
| 1:A:483:TYR:CD2  | 1:A:496:ARG:NH2  | 0.59     | 2.71        | 14     | 1     |
| 1:A:473:ASP:O    | 1:A:477:ALA:HB2  | 0.58     | 1.98        | 6      | 6     |
| 1:A:457:VAL:O    | 1:A:457:VAL:HG13 | 0.58     | 1.99        | 5      | 2     |
| 1:A:463:GLU:N    | 1:A:464:PRO:CD   | 0.58     | 2.66        | 20     | 19    |
| 1:A:496:ARG:HH11 | 1:A:536:ILE:HD13 | 0.58     | 1.59        | 2      | 1     |
| 1:A:462:THR:HG23 | 1:A:520:LYS:NZ   | 0.58     | 2.13        | 20     | 1     |
| 1:A:455:VAL:HG21 | 1:A:499:THR:O    | 0.58     | 1.98        | 13     | 5     |
| 1:A:516:LYS:CG   | 1:A:517:HIS:NE2  | 0.58     | 2.67        | 2      | 7     |
| 1:A:478:ILE:CG2  | 1:A:506:VAL:HG23 | 0.58     | 2.29        | 7      | 2     |
| 1:A:532:TYR:CD2  | 1:A:535:LYS:CE   | 0.58     | 2.87        | 18     | 2     |
| 1:A:507:ILE:CG2  | 1:A:521:LEU:HD21 | 0.58     | 2.29        | 2      | 2     |
| 1:A:478:ILE:HG21 | 1:A:506:VAL:HA   | 0.58     | 1.76        | 6      | 6     |
| 1:A:465:LEU:HD13 | 1:A:491:THR:O    | 0.57     | 1.98        | 2      | 8     |
| 1:A:478:ILE:HG21 | 1:A:506:VAL:HG23 | 0.57     | 1.76        | 13     | 2     |
| 1:A:475:LEU:HD12 | 1:A:476:ALA:N    | 0.57     | 2.14        | 20     | 9     |
| 1:A:486:LEU:HD22 | 1:A:486:LEU:C    | 0.57     | 2.22        | 15     | 3     |
| 1:A:472:ARG:HB2  | 1:A:484:VAL:HG21 | 0.57     | 1.76        | 13     | 2     |
| 1:A:532:TYR:CE2  | 1:A:535:LYS:HE2  | 0.57     | 2.35        | 5      | 5     |
| 1:A:472:ARG:HA   | 1:A:484:VAL:HG21 | 0.57     | 1.76        | 7      | 3     |
| 1:A:466:PRO:CG   | 1:A:470:GLN:CB   | 0.57     | 2.82        | 18     | 14    |
| 1:A:486:LEU:HD12 | 1:A:493:CYS:CB   | 0.57     | 2.30        | 1      | 5     |
| 1:A:482:LEU:HD12 | 1:A:498:LYS:HG3  | 0.57     | 1.75        | 2      | 1     |
| 1:A:456:ILE:HD11 | 1:A:533:TRP:NE1  | 0.57     | 2.15        | 17     | 1     |
| 1:A:516:LYS:C    | 1:A:517:HIS:CG   | 0.57     | 2.83        | 13     | 11    |
| 1:A:478:ILE:CG2  | 1:A:506:VAL:HG22 | 0.56     | 2.30        | 8      | 1     |
| 1:A:465:LEU:HD23 | 1:A:471:VAL:HG21 | 0.56     | 1.76        | 20     | 1     |
| 1:A:516:LYS:HG3  | 1:A:517:HIS:CE1  | 0.56     | 2.35        | 9      | 5     |
| 1:A:532:TYR:CD2  | 1:A:535:LYS:HE2  | 0.56     | 2.35        | 18     | 4     |
| 1:A:475:LEU:HD13 | 1:A:481:VAL:HG11 | 0.56     | 1.78        | 11     | 8     |
| 1:A:487:LEU:N    | 1:A:487:LEU:CD2  | 0.56     | 2.68        | 11     | 1     |
| 1:A:462:THR:O    | 1:A:463:GLU:CB   | 0.56     | 2.53        | 11     | 20    |
| 1:A:467:GLY:O    | 1:A:470:GLN:N    | 0.56     | 2.38        | 9      | 1     |
| 1:A:497:PHE:HE1  | 1:A:506:VAL:HG21 | 0.56     | 1.61        | 16     | 1     |
| 1:A:472:ARG:O    | 1:A:476:ALA:HB3  | 0.56     | 2.01        | 6      | 4     |
| 1:A:486:LEU:HD23 | 1:A:493:CYS:HB3  | 0.56     | 1.76        | 2      | 2     |
| 1:A:483:TYR:C    | 1:A:483:TYR:CD1  | 0.56     | 2.84        | 7      | 8     |
| 1:A:487:LEU:HD13 | 1:A:492:GLU:HG3  | 0.56     | 1.76        | 9      | 2     |
| 1:A:510:TYR:CE1  | 1:A:521:LEU:CD2  | 0.55     | 2.88        | 20     | 1     |
| 1:A:457:VAL:CG1  | 1:A:521:LEU:HD21 | 0.55     | 2.31        | 19     | 3     |
| 1:A:471:VAL:HG22 | 1:A:519:TRP:CH2  | 0.55     | 2.36        | 11     | 8     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:516:LYS:CD   | 1:A:517:HIS:CE1  | 0.55     | 2.89        | 6      | 2     |
| 1:A:503:ALA:O    | 1:A:506:VAL:HG12 | 0.55     | 2.02        | 17     | 11    |
| 1:A:516:LYS:HD3  | 1:A:517:HIS:CE1  | 0.55     | 2.37        | 19     | 2     |
| 1:A:486:LEU:HD12 | 1:A:487:LEU:H    | 0.55     | 1.60        | 10     | 1     |
| 1:A:483:TYR:CE1  | 1:A:485:ASP:OD2  | 0.55     | 2.59        | 16     | 1     |
| 1:A:474:THR:O    | 1:A:477:ALA:N    | 0.55     | 2.40        | 3      | 11    |
| 1:A:475:LEU:HD11 | 1:A:481:VAL:HG21 | 0.55     | 1.77        | 18     | 4     |
| 1:A:507:ILE:HG22 | 1:A:521:LEU:CD1  | 0.55     | 2.32        | 7      | 1     |
| 1:A:455:VAL:HG21 | 1:A:497:PHE:O    | 0.54     | 2.01        | 14     | 3     |
| 1:A:456:ILE:HD12 | 1:A:532:TYR:CE1  | 0.54     | 2.37        | 15     | 1     |
| 1:A:507:ILE:HG21 | 1:A:523:ILE:HD11 | 0.54     | 1.78        | 18     | 1     |
| 1:A:510:TYR:CE1  | 1:A:521:LEU:HD22 | 0.54     | 2.36        | 11     | 1     |
| 1:A:483:TYR:CE1  | 1:A:484:VAL:O    | 0.54     | 2.61        | 6      | 1     |
| 1:A:468:ARG:HB3  | 1:A:486:LEU:HD22 | 0.54     | 1.78        | 4      | 1     |
| 1:A:481:VAL:HG12 | 1:A:497:PHE:CD1  | 0.54     | 2.37        | 18     | 4     |
| 1:A:483:TYR:CD2  | 1:A:483:TYR:C    | 0.54     | 2.86        | 4      | 7     |
| 1:A:510:TYR:CD1  | 1:A:521:LEU:HG   | 0.54     | 2.38        | 20     | 4     |
| 1:A:521:LEU:N    | 1:A:521:LEU:CD2  | 0.54     | 2.71        | 18     | 6     |
| 1:A:458:LYS:HB2  | 1:A:524:LEU:HD21 | 0.53     | 1.80        | 10     | 3     |
| 1:A:503:ALA:O    | 1:A:506:VAL:CG1  | 0.53     | 2.56        | 17     | 7     |
| 1:A:478:ILE:HG13 | 1:A:510:TYR:CE2  | 0.53     | 2.39        | 19     | 1     |
| 1:A:472:ARG:O    | 1:A:476:ALA:CB   | 0.53     | 2.56        | 6      | 8     |
| 1:A:455:VAL:CB   | 1:A:497:PHE:O    | 0.53     | 2.56        | 18     | 5     |
| 1:A:457:VAL:O    | 1:A:457:VAL:CG1  | 0.53     | 2.56        | 5      | 2     |
| 1:A:507:ILE:HG12 | 1:A:523:ILE:HD11 | 0.53     | 1.81        | 14     | 2     |
| 1:A:486:LEU:C    | 1:A:486:LEU:HD13 | 0.52     | 2.28        | 15     | 2     |
| 1:A:460:ILE:CG2  | 1:A:520:LYS:HB2  | 0.52     | 2.34        | 13     | 19    |
| 1:A:496:ARG:HD2  | 1:A:533:TRP:CH2  | 0.52     | 2.40        | 10     | 5     |
| 1:A:510:TYR:CD1  | 1:A:521:LEU:CD2  | 0.52     | 2.92        | 20     | 1     |
| 1:A:471:VAL:O    | 1:A:475:LEU:CD2  | 0.52     | 2.57        | 8      | 2     |
| 1:A:487:LEU:O    | 1:A:490:ASP:N    | 0.52     | 2.43        | 13     | 15    |
| 1:A:466:PRO:HG2  | 1:A:470:GLN:CB   | 0.52     | 2.34        | 11     | 13    |
| 1:A:484:VAL:O    | 1:A:484:VAL:CG1  | 0.52     | 2.58        | 18     | 3     |
| 1:A:463:GLU:N    | 1:A:464:PRO:HD2  | 0.52     | 2.20        | 11     | 19    |
| 1:A:534:GLN:O    | 1:A:538:VAL:CG2  | 0.52     | 2.58        | 2      | 3     |
| 1:A:516:LYS:HG2  | 1:A:517:HIS:CE1  | 0.52     | 2.39        | 4      | 1     |
| 1:A:480:GLU:O    | 1:A:480:GLU:CG   | 0.52     | 2.57        | 12     | 1     |
| 1:A:496:ARG:CZ   | 1:A:536:ILE:HD13 | 0.52     | 2.35        | 19     | 1     |
| 1:A:461:SER:HB2  | 1:A:519:TRP:CD1  | 0.51     | 2.40        | 1      | 4     |
| 1:A:484:VAL:HG13 | 1:A:495:ALA:CB   | 0.51     | 2.30        | 3      | 1     |
| 1:A:504:GLN:OE1  | 1:A:508:ASN:ND2  | 0.51     | 2.43        | 3      | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:517:HIS:O    | 1:A:519:TRP:N    | 0.51     | 2.43        | 13     | 2     |
| 1:A:466:PRO:CG   | 1:A:470:GLN:HB3  | 0.51     | 2.35        | 7      | 11    |
| 1:A:460:ILE:CD1  | 1:A:461:SER:O    | 0.51     | 2.57        | 9      | 5     |
| 1:A:457:VAL:CG1  | 1:A:521:LEU:CD1  | 0.51     | 2.87        | 17     | 1     |
| 1:A:510:TYR:CD1  | 1:A:521:LEU:HD23 | 0.51     | 2.40        | 20     | 1     |
| 1:A:462:THR:O    | 1:A:463:GLU:CG   | 0.51     | 2.58        | 13     | 12    |
| 1:A:529:GLU:OE1  | 1:A:533:TRP:CD1  | 0.51     | 2.63        | 13     | 1     |
| 1:A:461:SER:OG   | 1:A:462:THR:N    | 0.51     | 2.43        | 14     | 3     |
| 1:A:513:ILE:HG21 | 1:A:519:TRP:HB2  | 0.51     | 1.82        | 4      | 5     |
| 1:A:521:LEU:CG   | 1:A:521:LEU:O    | 0.51     | 2.58        | 14     | 1     |
| 1:A:531:ARG:CD   | 1:A:531:ARG:C    | 0.51     | 2.82        | 6      | 5     |
| 1:A:507:ILE:HG22 | 1:A:521:LEU:HD12 | 0.51     | 1.81        | 17     | 2     |
| 1:A:464:PRO:O    | 1:A:465:LEU:C    | 0.51     | 2.54        | 12     | 18    |
| 1:A:467:GLY:O    | 1:A:471:VAL:CG2  | 0.51     | 2.58        | 16     | 5     |
| 1:A:485:ASP:O    | 1:A:493:CYS:CB   | 0.51     | 2.58        | 19     | 1     |
| 1:A:510:TYR:CG   | 1:A:513:ILE:HG13 | 0.51     | 2.40        | 19     | 2     |
| 1:A:467:GLY:O    | 1:A:468:ARG:C    | 0.51     | 2.53        | 9      | 1     |
| 1:A:461:SER:OG   | 1:A:465:LEU:CD1  | 0.50     | 2.57        | 8      | 5     |
| 1:A:524:LEU:CD1  | 1:A:528:HIS:ND1  | 0.50     | 2.74        | 15     | 1     |
| 1:A:482:LEU:C    | 1:A:482:LEU:CD1  | 0.50     | 2.84        | 20     | 1     |
| 1:A:507:ILE:CA   | 1:A:521:LEU:HD23 | 0.50     | 2.31        | 1      | 2     |
| 1:A:486:LEU:HD22 | 1:A:487:LEU:H    | 0.50     | 1.60        | 15     | 2     |
| 1:A:510:TYR:O    | 1:A:513:ILE:CG1  | 0.50     | 2.59        | 19     | 1     |
| 1:A:485:ASP:CB   | 1:A:494:HIS:O    | 0.50     | 2.59        | 4      | 1     |
| 1:A:521:LEU:O    | 1:A:521:LEU:CD2  | 0.50     | 2.60        | 7      | 1     |
| 1:A:518:CYS:O    | 1:A:520:LYS:NZ   | 0.50     | 2.44        | 8      | 1     |
| 1:A:487:LEU:O    | 1:A:488:GLU:C    | 0.50     | 2.54        | 8      | 16    |
| 1:A:513:ILE:HG21 | 1:A:519:TRP:CB   | 0.50     | 2.36        | 7      | 4     |
| 1:A:524:LEU:CD2  | 1:A:524:LEU:N    | 0.50     | 2.75        | 2      | 1     |
| 1:A:475:LEU:CD1  | 1:A:481:VAL:CG2  | 0.50     | 2.85        | 14     | 1     |
| 1:A:507:ILE:CA   | 1:A:521:LEU:HD21 | 0.50     | 2.37        | 14     | 2     |
| 1:A:516:LYS:HG3  | 1:A:517:HIS:NE2  | 0.50     | 2.21        | 8      | 6     |
| 1:A:521:LEU:CD2  | 1:A:521:LEU:O    | 0.50     | 2.59        | 14     | 1     |
| 1:A:532:TYR:CG   | 1:A:535:LYS:HE3  | 0.50     | 2.41        | 18     | 1     |
| 1:A:482:LEU:HD12 | 1:A:498:LYS:HB3  | 0.50     | 1.82        | 10     | 1     |
| 1:A:508:ASN:O    | 1:A:511:THR:HG22 | 0.49     | 2.07        | 14     | 5     |
| 1:A:482:LEU:HD13 | 1:A:498:LYS:HG3  | 0.49     | 1.84        | 18     | 1     |
| 1:A:456:ILE:HG22 | 1:A:524:LEU:HD23 | 0.49     | 1.84        | 7      | 1     |
| 1:A:516:LYS:HG2  | 1:A:517:HIS:NE2  | 0.49     | 2.22        | 5      | 6     |
| 1:A:455:VAL:CG2  | 1:A:497:PHE:O    | 0.49     | 2.60        | 14     | 3     |
| 1:A:516:LYS:O    | 1:A:517:HIS:CG   | 0.49     | 2.66        | 12     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:472:ARG:HG3  | 1:A:473:ASP:N    | 0.49     | 2.23        | 9      | 8     |
| 1:A:455:VAL:HG12 | 1:A:499:THR:C    | 0.49     | 2.32        | 5      | 2     |
| 1:A:485:ASP:OD2  | 1:A:485:ASP:N    | 0.49     | 2.46        | 13     | 1     |
| 1:A:464:PRO:O    | 1:A:466:PRO:N    | 0.49     | 2.46        | 12     | 5     |
| 1:A:524:LEU:HD13 | 1:A:528:HIS:ND1  | 0.49     | 2.23        | 15     | 1     |
| 1:A:504:GLN:O    | 1:A:508:ASN:ND2  | 0.49     | 2.45        | 8      | 12    |
| 1:A:478:ILE:HG21 | 1:A:506:VAL:HG13 | 0.49     | 1.83        | 2      | 1     |
| 1:A:478:ILE:HB   | 1:A:506:VAL:HG23 | 0.49     | 1.83        | 19     | 2     |
| 1:A:475:LEU:HD11 | 1:A:484:VAL:CG2  | 0.49     | 2.38        | 7      | 1     |
| 1:A:530:GLN:CD   | 1:A:530:GLN:C    | 0.49     | 2.81        | 17     | 4     |
| 1:A:466:PRO:HB2  | 1:A:470:GLN:CB   | 0.49     | 2.37        | 16     | 4     |
| 1:A:494:HIS:CD2  | 1:A:532:TYR:CE2  | 0.49     | 3.01        | 8      | 2     |
| 1:A:512:GLU:O    | 1:A:515:LYS:CG   | 0.48     | 2.61        | 10     | 3     |
| 1:A:510:TYR:CD1  | 1:A:521:LEU:HB3  | 0.48     | 2.43        | 14     | 2     |
| 1:A:516:LYS:HB3  | 1:A:517:HIS:CD2  | 0.48     | 2.44        | 6      | 9     |
| 1:A:465:LEU:CD1  | 1:A:491:THR:O    | 0.48     | 2.61        | 2      | 3     |
| 1:A:516:LYS:CG   | 1:A:517:HIS:CE1  | 0.48     | 2.97        | 9      | 1     |
| 1:A:473:ASP:O    | 1:A:477:ALA:CB   | 0.48     | 2.61        | 14     | 3     |
| 1:A:513:ILE:HG21 | 1:A:519:TRP:HB3  | 0.48     | 1.84        | 7      | 2     |
| 1:A:514:ASN:ND2  | 1:A:518:CYS:SG   | 0.48     | 2.86        | 8      | 1     |
| 1:A:513:ILE:HD13 | 1:A:519:TRP:CE3  | 0.48     | 2.43        | 17     | 1     |
| 1:A:532:TYR:CD1  | 1:A:535:LYS:HE3  | 0.48     | 2.44        | 18     | 1     |
| 1:A:466:PRO:HB2  | 1:A:470:GLN:CG   | 0.48     | 2.39        | 4      | 1     |
| 1:A:494:HIS:HB2  | 1:A:532:TYR:CZ   | 0.48     | 2.44        | 13     | 2     |
| 1:A:460:ILE:HD12 | 1:A:491:THR:O    | 0.47     | 2.09        | 1      | 1     |
| 1:A:466:PRO:CB   | 1:A:470:GLN:CB   | 0.47     | 2.92        | 16     | 1     |
| 1:A:504:GLN:O    | 1:A:507:ILE:HG13 | 0.47     | 2.09        | 7      | 20    |
| 1:A:456:ILE:HG21 | 1:A:532:TYR:CG   | 0.47     | 2.44        | 14     | 1     |
| 1:A:459:ILE:HD13 | 1:A:521:LEU:HD21 | 0.47     | 1.86        | 17     | 1     |
| 1:A:482:LEU:O    | 1:A:483:TYR:CB   | 0.47     | 2.61        | 4      | 1     |
| 1:A:455:VAL:HB   | 1:A:497:PHE:O    | 0.47     | 2.10        | 18     | 5     |
| 1:A:510:TYR:CE1  | 1:A:519:TRP:CE3  | 0.47     | 3.02        | 18     | 2     |
| 1:A:510:TYR:CD1  | 1:A:521:LEU:CG   | 0.47     | 2.98        | 10     | 2     |
| 1:A:507:ILE:HD12 | 1:A:507:ILE:C    | 0.47     | 2.34        | 12     | 1     |
| 1:A:479:SER:HB3  | 1:A:506:VAL:CG2  | 0.47     | 2.39        | 2      | 1     |
| 1:A:526:GLY:O    | 1:A:529:GLU:N    | 0.47     | 2.48        | 5      | 5     |
| 1:A:486:LEU:CD2  | 1:A:493:CYS:HB3  | 0.47     | 2.39        | 8      | 1     |
| 1:A:489:GLY:O    | 1:A:490:ASP:O    | 0.47     | 2.32        | 10     | 2     |
| 1:A:508:ASN:O    | 1:A:511:THR:HG23 | 0.47     | 2.09        | 6      | 2     |
| 1:A:479:SER:O    | 1:A:480:GLU:C    | 0.47     | 2.57        | 14     | 1     |
| 1:A:456:ILE:HG12 | 1:A:533:TRP:NE1  | 0.47     | 2.25        | 13     | 7     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:535:LYS:HD2  | 1:A:536:ILE:N    | 0.47     | 2.24        | 1      | 3     |
| 1:A:529:GLU:CG   | 1:A:530:GLN:N    | 0.47     | 2.78        | 18     | 7     |
| 1:A:456:ILE:O    | 1:A:524:LEU:HD23 | 0.47     | 2.10        | 7      | 1     |
| 1:A:486:LEU:O    | 1:A:488:GLU:N    | 0.46     | 2.48        | 7      | 1     |
| 1:A:471:VAL:O    | 1:A:474:THR:OG1  | 0.46     | 2.30        | 17     | 11    |
| 1:A:532:TYR:C    | 1:A:532:TYR:CD1  | 0.46     | 2.93        | 5      | 1     |
| 1:A:516:LYS:HA   | 1:A:516:LYS:CE   | 0.46     | 2.41        | 18     | 4     |
| 1:A:484:VAL:HG22 | 1:A:495:ALA:CB   | 0.46     | 2.40        | 15     | 1     |
| 1:A:459:ILE:HG21 | 1:A:519:TRP:CZ2  | 0.46     | 2.45        | 3      | 2     |
| 1:A:475:LEU:N    | 1:A:510:TYR:OH   | 0.46     | 2.48        | 3      | 2     |
| 1:A:512:GLU:O    | 1:A:513:ILE:C    | 0.46     | 2.59        | 18     | 7     |
| 1:A:482:LEU:O    | 1:A:483:TYR:HB2  | 0.46     | 2.11        | 4      | 2     |
| 1:A:468:ARG:CA   | 1:A:486:LEU:HD13 | 0.46     | 2.40        | 9      | 1     |
| 1:A:487:LEU:O    | 1:A:490:ASP:CB   | 0.46     | 2.63        | 17     | 2     |
| 1:A:486:LEU:HD13 | 1:A:486:LEU:O    | 0.46     | 2.11        | 16     | 2     |
| 1:A:483:TYR:CD1  | 1:A:483:TYR:C    | 0.46     | 2.93        | 2      | 2     |
| 1:A:521:LEU:O    | 1:A:521:LEU:CG   | 0.46     | 2.63        | 7      | 1     |
| 1:A:478:ILE:HG13 | 1:A:510:TYR:CD2  | 0.46     | 2.45        | 19     | 1     |
| 1:A:479:SER:CB   | 1:A:506:VAL:CG2  | 0.46     | 2.94        | 2      | 1     |
| 1:A:481:VAL:HG12 | 1:A:497:PHE:CZ   | 0.46     | 2.45        | 5      | 1     |
| 1:A:499:THR:OG1  | 1:A:502:ASP:OD2  | 0.46     | 2.33        | 8      | 2     |
| 1:A:530:GLN:OE1  | 1:A:534:GLN:CG   | 0.46     | 2.64        | 16     | 2     |
| 1:A:464:PRO:O    | 1:A:465:LEU:O    | 0.46     | 2.34        | 16     | 1     |
| 1:A:472:ARG:HA   | 1:A:475:LEU:HD21 | 0.46     | 1.87        | 2      | 1     |
| 1:A:455:VAL:HG23 | 1:A:497:PHE:O    | 0.46     | 2.10        | 3      | 2     |
| 1:A:486:LEU:HA   | 1:A:493:CYS:CB   | 0.46     | 2.41        | 7      | 2     |
| 1:A:482:LEU:HD23 | 1:A:496:ARG:HB2  | 0.46     | 1.87        | 4      | 1     |
| 1:A:524:LEU:N    | 1:A:524:LEU:HD23 | 0.45     | 2.25        | 2      | 1     |
| 1:A:532:TYR:CD1  | 1:A:532:TYR:C    | 0.45     | 2.94        | 18     | 2     |
| 1:A:482:LEU:HD12 | 1:A:482:LEU:O    | 0.45     | 2.10        | 20     | 1     |
| 1:A:501:GLU:CD   | 1:A:502:ASP:N    | 0.45     | 2.74        | 5      | 1     |
| 1:A:487:LEU:HD22 | 1:A:492:GLU:HG3  | 0.45     | 1.88        | 7      | 1     |
| 1:A:487:LEU:HB3  | 1:A:490:ASP:CB   | 0.45     | 2.41        | 14     | 5     |
| 1:A:492:GLU:CG   | 1:A:492:GLU:O    | 0.45     | 2.63        | 10     | 1     |
| 1:A:486:LEU:CD1  | 1:A:493:CYS:HB2  | 0.45     | 2.40        | 4      | 4     |
| 1:A:507:ILE:HA   | 1:A:521:LEU:HD13 | 0.45     | 1.87        | 19     | 3     |
| 1:A:521:LEU:HG   | 1:A:521:LEU:O    | 0.45     | 2.12        | 14     | 1     |
| 1:A:473:ASP:OD1  | 1:A:473:ASP:C    | 0.45     | 2.60        | 15     | 1     |
| 1:A:471:VAL:HA   | 1:A:474:THR:OG1  | 0.45     | 2.12        | 5      | 3     |
| 1:A:501:GLU:HG3  | 1:A:502:ASP:N    | 0.45     | 2.26        | 1      | 1     |
| 1:A:478:ILE:CB   | 1:A:506:VAL:HG23 | 0.45     | 2.42        | 3      | 1     |

Continued on next page...

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:455:VAL:HG12 | 1:A:500:PRO:N    | 0.45     | 2.27        | 5      | 1     |
| 1:A:456:ILE:CD1  | 1:A:496:ARG:HB3  | 0.45     | 2.42        | 12     | 3     |
| 1:A:468:ARG:HG3  | 1:A:469:LYS:N    | 0.45     | 2.26        | 15     | 1     |
| 1:A:526:GLY:C    | 1:A:528:HIS:N    | 0.45     | 2.74        | 5      | 5     |
| 1:A:497:PHE:N    | 1:A:497:PHE:CD1  | 0.45     | 2.84        | 14     | 3     |
| 1:A:516:LYS:CG   | 1:A:517:HIS:CD2  | 0.45     | 3.00        | 8      | 1     |
| 1:A:475:LEU:HD13 | 1:A:481:VAL:HG21 | 0.45     | 1.86        | 14     | 1     |
| 1:A:466:PRO:HB2  | 1:A:470:GLN:HB2  | 0.45     | 1.89        | 16     | 1     |
| 1:A:513:ILE:HD13 | 1:A:519:TRP:HE3  | 0.45     | 1.72        | 17     | 1     |
| 1:A:459:ILE:CG2  | 1:A:519:TRP:CE2  | 0.45     | 2.99        | 3      | 1     |
| 1:A:456:ILE:O    | 1:A:456:ILE:HG22 | 0.45     | 2.12        | 16     | 1     |
| 1:A:483:TYR:CD1  | 1:A:485:ASP:OD2  | 0.45     | 2.70        | 16     | 1     |
| 1:A:485:ASP:OD2  | 1:A:532:TYR:OH   | 0.45     | 2.35        | 2      | 1     |
| 1:A:510:TYR:CG   | 1:A:521:LEU:HD13 | 0.45     | 2.43        | 2      | 1     |
| 1:A:530:GLN:HG3  | 1:A:531:ARG:N    | 0.45     | 2.27        | 18     | 6     |
| 1:A:526:GLY:O    | 1:A:527:ASP:C    | 0.45     | 2.58        | 5      | 7     |
| 1:A:456:ILE:O    | 1:A:524:LEU:CD2  | 0.45     | 2.65        | 7      | 1     |
| 1:A:494:HIS:HB2  | 1:A:532:TYR:OH   | 0.45     | 2.11        | 8      | 1     |
| 1:A:507:ILE:HG21 | 1:A:523:ILE:CD1  | 0.44     | 2.42        | 2      | 1     |
| 1:A:485:ASP:HB2  | 1:A:496:ARG:NH1  | 0.44     | 2.27        | 14     | 1     |
| 1:A:465:LEU:CD2  | 1:A:471:VAL:CG2  | 0.44     | 2.95        | 8      | 2     |
| 1:A:518:CYS:SG   | 1:A:520:LYS:CE   | 0.44     | 3.06        | 6      | 2     |
| 1:A:535:LYS:HG2  | 1:A:536:ILE:N    | 0.44     | 2.27        | 18     | 3     |
| 1:A:469:LYS:HG3  | 1:A:470:GLN:N    | 0.44     | 2.28        | 8      | 1     |
| 1:A:535:LYS:O    | 1:A:539:ASP:HB2  | 0.44     | 2.12        | 19     | 3     |
| 1:A:465:LEU:O    | 1:A:466:PRO:C    | 0.44     | 2.61        | 16     | 1     |
| 1:A:485:ASP:OD1  | 1:A:494:HIS:O    | 0.44     | 2.35        | 16     | 1     |
| 1:A:470:GLN:O    | 1:A:474:THR:OG1  | 0.44     | 2.33        | 1      | 2     |
| 1:A:483:TYR:CD1  | 1:A:484:VAL:N    | 0.44     | 2.85        | 3      | 3     |
| 1:A:486:LEU:CG   | 1:A:493:CYS:HB3  | 0.44     | 2.43        | 8      | 1     |
| 1:A:460:ILE:O    | 1:A:520:LYS:HG2  | 0.44     | 2.12        | 10     | 11    |
| 1:A:518:CYS:SG   | 1:A:518:CYS:O    | 0.44     | 2.76        | 3      | 1     |
| 1:A:526:GLY:O    | 1:A:528:HIS:N    | 0.44     | 2.51        | 5      | 3     |
| 1:A:472:ARG:CB   | 1:A:484:VAL:HG11 | 0.44     | 2.42        | 1      | 3     |
| 1:A:464:PRO:O    | 1:A:466:PRO:CD   | 0.44     | 2.66        | 2      | 3     |
| 1:A:485:ASP:HB3  | 1:A:494:HIS:O    | 0.44     | 2.12        | 4      | 1     |
| 1:A:466:PRO:HG2  | 1:A:470:GLN:HB3  | 0.44     | 1.89        | 10     | 3     |
| 1:A:484:VAL:HG22 | 1:A:495:ALA:HB1  | 0.44     | 1.89        | 15     | 1     |
| 1:A:535:LYS:O    | 1:A:539:ASP:CB   | 0.44     | 2.66        | 15     | 2     |
| 1:A:530:GLN:OE1  | 1:A:534:GLN:HG2  | 0.44     | 2.12        | 16     | 1     |
| 1:A:480:GLU:O    | 1:A:480:GLU:HG3  | 0.44     | 2.12        | 12     | 1     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:466:PRO:HB2  | 1:A:470:GLN:CD   | 0.44     | 2.38        | 14     | 1     |
| 1:A:535:LYS:CD   | 1:A:535:LYS:C    | 0.43     | 2.90        | 12     | 2     |
| 1:A:497:PHE:N    | 1:A:497:PHE:CD2  | 0.43     | 2.86        | 8      | 4     |
| 1:A:503:ALA:O    | 1:A:507:ILE:HG12 | 0.43     | 2.13        | 8      | 1     |
| 1:A:487:LEU:CD1  | 1:A:492:GLU:O    | 0.43     | 2.66        | 12     | 1     |
| 1:A:463:GLU:O    | 1:A:465:LEU:N    | 0.43     | 2.51        | 19     | 1     |
| 1:A:510:TYR:CE1  | 1:A:521:LEU:HD23 | 0.43     | 2.47        | 20     | 1     |
| 1:A:471:VAL:HG13 | 1:A:519:TRP:HH2  | 0.43     | 1.73        | 16     | 1     |
| 1:A:536:ILE:CG2  | 1:A:540:ARG:NH1  | 0.43     | 2.81        | 18     | 1     |
| 1:A:457:VAL:HG13 | 1:A:521:LEU:CD1  | 0.43     | 2.43        | 20     | 1     |
| 1:A:532:TYR:CZ   | 1:A:535:LYS:HE3  | 0.43     | 2.47        | 17     | 4     |
| 1:A:522:GLU:OE2  | 1:A:523:ILE:O    | 0.43     | 2.37        | 3      | 1     |
| 1:A:532:TYR:CE2  | 1:A:535:LYS:NZ   | 0.43     | 2.84        | 6      | 1     |
| 1:A:461:SER:HB3  | 1:A:519:TRP:NE1  | 0.43     | 2.28        | 7      | 3     |
| 1:A:487:LEU:HD22 | 1:A:492:GLU:HG2  | 0.43     | 1.87        | 7      | 1     |
| 1:A:486:LEU:C    | 1:A:486:LEU:CD1  | 0.43     | 2.87        | 2      | 1     |
| 1:A:510:TYR:O    | 1:A:513:ILE:HG12 | 0.43     | 2.14        | 7      | 3     |
| 1:A:471:VAL:HG12 | 1:A:475:LEU:CD2  | 0.43     | 2.43        | 8      | 1     |
| 1:A:530:GLN:O    | 1:A:534:GLN:HG3  | 0.43     | 2.13        | 9      | 1     |
| 1:A:458:LYS:HG3  | 1:A:494:HIS:CE1  | 0.43     | 2.49        | 11     | 1     |
| 1:A:461:SER:HB2  | 1:A:519:TRP:NE1  | 0.43     | 2.29        | 10     | 4     |
| 1:A:466:PRO:HG2  | 1:A:470:GLN:HB2  | 0.43     | 1.91        | 7      | 4     |
| 1:A:456:ILE:HG13 | 1:A:532:TYR:CD1  | 0.43     | 2.49        | 18     | 3     |
| 1:A:462:THR:O    | 1:A:463:GLU:HB2  | 0.43     | 2.14        | 18     | 5     |
| 1:A:469:LYS:O    | 1:A:472:ARG:HG2  | 0.43     | 2.14        | 19     | 5     |
| 1:A:466:PRO:O    | 1:A:470:GLN:OE1  | 0.43     | 2.36        | 9      | 1     |
| 1:A:516:LYS:O    | 1:A:517:HIS:ND1  | 0.43     | 2.52        | 12     | 1     |
| 1:A:512:GLU:HG3  | 1:A:513:ILE:N    | 0.43     | 2.29        | 15     | 1     |
| 1:A:513:ILE:O    | 1:A:514:ASN:C    | 0.43     | 2.62        | 17     | 1     |
| 1:A:512:GLU:O    | 1:A:515:LYS:HG2  | 0.42     | 2.14        | 15     | 2     |
| 1:A:465:LEU:HD13 | 1:A:491:THR:C    | 0.42     | 2.38        | 19     | 2     |
| 1:A:458:LYS:HG3  | 1:A:494:HIS:NE2  | 0.42     | 2.29        | 11     | 4     |
| 1:A:468:ARG:N    | 1:A:486:LEU:HD13 | 0.42     | 2.29        | 9      | 1     |
| 1:A:512:GLU:O    | 1:A:515:LYS:N    | 0.42     | 2.44        | 19     | 2     |
| 1:A:492:GLU:N    | 1:A:492:GLU:OE2  | 0.42     | 2.52        | 19     | 1     |
| 1:A:468:ARG:HG2  | 1:A:469:LYS:N    | 0.42     | 2.29        | 20     | 1     |
| 1:A:536:ILE:O    | 1:A:537:LEU:C    | 0.42     | 2.62        | 20     | 1     |
| 1:A:460:ILE:HG23 | 1:A:520:LYS:HG3  | 0.42     | 1.91        | 6      | 4     |
| 1:A:516:LYS:CE   | 1:A:516:LYS:HA   | 0.42     | 2.44        | 11     | 2     |
| 1:A:466:PRO:HB3  | 1:A:470:GLN:HB3  | 0.42     | 1.92        | 9      | 1     |
| 1:A:471:VAL:HG22 | 1:A:519:TRP:HZ2  | 0.42     | 1.69        | 15     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:514:ASN:O    | 1:A:514:ASN:ND2  | 0.42     | 2.52        | 2      | 1     |
| 1:A:487:LEU:HD13 | 1:A:492:GLU:O    | 0.42     | 2.14        | 7      | 1     |
| 1:A:486:LEU:C    | 1:A:486:LEU:HD23 | 0.42     | 2.38        | 9      | 1     |
| 1:A:476:ALA:O    | 1:A:479:SER:O    | 0.42     | 2.38        | 10     | 1     |
| 1:A:485:ASP:OD2  | 1:A:496:ARG:CG   | 0.42     | 2.68        | 13     | 1     |
| 1:A:486:LEU:CD1  | 1:A:493:CYS:HB3  | 0.42     | 2.42        | 1      | 1     |
| 1:A:510:TYR:O    | 1:A:511:THR:C    | 0.42     | 2.63        | 12     | 1     |
| 1:A:525:SER:CA   | 1:A:529:GLU:HB3  | 0.42     | 2.45        | 12     | 1     |
| 1:A:486:LEU:CG   | 1:A:493:CYS:HB2  | 0.42     | 2.45        | 4      | 2     |
| 1:A:468:ARG:O    | 1:A:472:ARG:HB3  | 0.42     | 2.15        | 14     | 2     |
| 1:A:507:ILE:HG13 | 1:A:508:ASN:N    | 0.42     | 2.29        | 7      | 1     |
| 1:A:484:VAL:CG2  | 1:A:493:CYS:SG   | 0.42     | 3.07        | 16     | 1     |
| 1:A:535:LYS:CD   | 1:A:536:ILE:N    | 0.42     | 2.83        | 1      | 1     |
| 1:A:474:THR:O    | 1:A:475:LEU:C    | 0.42     | 2.62        | 15     | 5     |
| 1:A:503:ALA:O    | 1:A:507:ILE:CG1  | 0.42     | 2.68        | 8      | 1     |
| 1:A:457:VAL:O    | 1:A:494:HIS:HA   | 0.41     | 2.16        | 10     | 3     |
| 1:A:456:ILE:CG2  | 1:A:494:HIS:HB3  | 0.41     | 2.45        | 5      | 1     |
| 1:A:469:LYS:O    | 1:A:473:ASP:OD2  | 0.41     | 2.38        | 7      | 1     |
| 1:A:532:TYR:CD2  | 1:A:535:LYS:HE3  | 0.41     | 2.49        | 18     | 1     |
| 1:A:464:PRO:O    | 1:A:466:PRO:HD3  | 0.41     | 2.15        | 5      | 4     |
| 1:A:472:ARG:CG   | 1:A:473:ASP:N    | 0.41     | 2.83        | 6      | 3     |
| 1:A:486:LEU:CB   | 1:A:493:CYS:HB3  | 0.41     | 2.45        | 9      | 3     |
| 1:A:483:TYR:CE2  | 1:A:484:VAL:O    | 0.41     | 2.72        | 4      | 1     |
| 1:A:507:ILE:HG21 | 1:A:523:ILE:HG13 | 0.41     | 1.93        | 12     | 1     |
| 1:A:510:TYR:CD1  | 1:A:521:LEU:HD11 | 0.41     | 2.51        | 15     | 1     |
| 1:A:483:TYR:CD2  | 1:A:496:ARG:CZ   | 0.41     | 3.03        | 14     | 2     |
| 1:A:475:LEU:CD1  | 1:A:481:VAL:HG11 | 0.41     | 2.46        | 8      | 2     |
| 1:A:503:ALA:HB1  | 1:A:523:ILE:HD12 | 0.41     | 1.92        | 13     | 1     |
| 1:A:468:ARG:O    | 1:A:472:ARG:CB   | 0.41     | 2.69        | 14     | 1     |
| 1:A:524:LEU:CD1  | 1:A:528:HIS:CE1  | 0.41     | 3.04        | 15     | 1     |
| 1:A:460:ILE:CD1  | 1:A:492:GLU:HG2  | 0.41     | 2.46        | 1      | 1     |
| 1:A:532:TYR:CE2  | 1:A:535:LYS:HE3  | 0.41     | 2.50        | 2      | 2     |
| 1:A:510:TYR:CD2  | 1:A:513:ILE:HG13 | 0.41     | 2.51        | 20     | 1     |
| 1:A:486:LEU:HG   | 1:A:493:CYS:CB   | 0.41     | 2.46        | 8      | 1     |
| 1:A:458:LYS:HB2  | 1:A:494:HIS:CD2  | 0.41     | 2.50        | 14     | 1     |
| 1:A:482:LEU:HD12 | 1:A:498:LYS:HG2  | 0.41     | 1.92        | 2      | 1     |
| 1:A:468:ARG:CB   | 1:A:486:LEU:HD13 | 0.41     | 2.45        | 8      | 1     |
| 1:A:466:PRO:HB3  | 1:A:470:GLN:CB   | 0.41     | 2.46        | 9      | 1     |
| 1:A:468:ARG:CB   | 1:A:486:LEU:HD23 | 0.41     | 2.45        | 13     | 1     |
| 1:A:460:ILE:HG22 | 1:A:520:LYS:CB   | 0.41     | 2.39        | 15     | 2     |
| 1:A:487:LEU:CB   | 1:A:490:ASP:HB3  | 0.41     | 2.46        | 15     | 1     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:486:LEU:C    | 1:A:486:LEU:CD2  | 0.41     | 2.93        | 17     | 1     |
| 1:A:530:GLN:O    | 1:A:534:GLN:CG   | 0.41     | 2.69        | 18     | 1     |
| 1:A:469:LYS:CG   | 1:A:470:GLN:N    | 0.41     | 2.83        | 19     | 1     |
| 1:A:462:THR:CG2  | 1:A:520:LYS:NZ   | 0.41     | 2.83        | 20     | 1     |
| 1:A:514:ASN:C    | 1:A:516:LYS:N    | 0.41     | 2.78        | 20     | 2     |
| 1:A:475:LEU:HD12 | 1:A:481:VAL:HG11 | 0.41     | 1.93        | 8      | 1     |
| 1:A:457:VAL:HG13 | 1:A:521:LEU:CD2  | 0.40     | 2.47        | 10     | 1     |
| 1:A:476:ALA:HA   | 1:A:479:SER:O    | 0.40     | 2.17        | 15     | 2     |
| 1:A:524:LEU:CD1  | 1:A:528:HIS:CG   | 0.40     | 3.04        | 15     | 1     |
| 1:A:466:PRO:HB2  | 1:A:470:GLN:HG3  | 0.40     | 1.93        | 3      | 1     |
| 1:A:458:LYS:CB   | 1:A:524:LEU:HD21 | 0.40     | 2.46        | 6      | 1     |
| 1:A:487:LEU:HD12 | 1:A:487:LEU:N    | 0.40     | 2.31        | 7      | 1     |
| 1:A:510:TYR:CE1  | 1:A:521:LEU:CD1  | 0.40     | 2.99        | 7      | 1     |
| 1:A:524:LEU:HD12 | 1:A:528:HIS:CG   | 0.40     | 2.51        | 7      | 1     |
| 1:A:519:TRP:C    | 1:A:520:LYS:HE2  | 0.40     | 2.41        | 15     | 1     |
| 1:A:499:THR:HG1  | 1:A:502:ASP:CG   | 0.40     | 2.24        | 20     | 1     |
| 1:A:462:THR:O    | 1:A:463:GLU:HG3  | 0.40     | 2.16        | 10     | 1     |
| 1:A:510:TYR:CD1  | 1:A:521:LEU:HB2  | 0.40     | 2.52        | 11     | 1     |
| 1:A:475:LEU:HD12 | 1:A:481:VAL:CG2  | 0.40     | 2.46        | 18     | 1     |
| 1:A:515:LYS:HG3  | 1:A:516:LYS:N    | 0.40     | 2.31        | 1      | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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     | 86/125 (69%)    | 74±2 (86±2%) | 8±2 (10±2%) | 3±1 (4±1%) | 4           | 30 |
| All | All   | 1720/2500 (69%) | 1484 (86%)   | 168 (10%)   | 68 (4%)    | 4           | 30 |

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 463 | GLU  | 20             |
| 1   | A     | 455 | VAL  | 15             |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 474 | THR  | 9              |
| 1   | A     | 487 | LEU  | 7              |
| 1   | A     | 490 | ASP  | 3              |
| 1   | A     | 527 | ASP  | 3              |
| 1   | A     | 518 | CYS  | 3              |
| 1   | A     | 483 | TYR  | 2              |
| 1   | A     | 465 | LEU  | 2              |
| 1   | A     | 464 | PRO  | 2              |
| 1   | A     | 468 | ARG  | 1              |
| 1   | A     | 488 | GLU  | 1              |

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|-------------|----|
| 1   | A     | 77/110 (70%)    | 52±3 (68±4%) | 25±3 (32±4%) | 1           | 14 |
| All | All   | 1540/2200 (70%) | 1046 (68%)   | 494 (32%)    | 1           | 14 |

All 59 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 465 | LEU  | 20             |
| 1   | A     | 510 | TYR  | 20             |
| 1   | A     | 516 | LYS  | 20             |
| 1   | A     | 535 | LYS  | 17             |
| 1   | A     | 499 | THR  | 16             |
| 1   | A     | 460 | ILE  | 16             |
| 1   | A     | 521 | LEU  | 16             |
| 1   | A     | 455 | VAL  | 15             |
| 1   | A     | 486 | LEU  | 15             |
| 1   | A     | 528 | HIS  | 14             |
| 1   | A     | 474 | THR  | 13             |
| 1   | A     | 517 | HIS  | 13             |
| 1   | A     | 498 | LYS  | 12             |
| 1   | A     | 519 | TRP  | 12             |
| 1   | A     | 482 | LEU  | 12             |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 463 | GLU  | 11             |
| 1   | A     | 537 | LEU  | 11             |
| 1   | A     | 520 | LYS  | 11             |
| 1   | A     | 496 | ARG  | 11             |
| 1   | A     | 487 | LEU  | 10             |
| 1   | A     | 515 | LYS  | 10             |
| 1   | A     | 530 | GLN  | 10             |
| 1   | A     | 469 | LYS  | 9              |
| 1   | A     | 479 | SER  | 9              |
| 1   | A     | 531 | ARG  | 9              |
| 1   | A     | 522 | GLU  | 9              |
| 1   | A     | 488 | GLU  | 8              |
| 1   | A     | 540 | ARG  | 8              |
| 1   | A     | 478 | ILE  | 8              |
| 1   | A     | 475 | LEU  | 7              |
| 1   | A     | 480 | GLU  | 7              |
| 1   | A     | 493 | CYS  | 7              |
| 1   | A     | 492 | GLU  | 7              |
| 1   | A     | 502 | ASP  | 7              |
| 1   | A     | 473 | ASP  | 6              |
| 1   | A     | 525 | SER  | 6              |
| 1   | A     | 468 | ARG  | 6              |
| 1   | A     | 504 | GLN  | 6              |
| 1   | A     | 507 | ILE  | 6              |
| 1   | A     | 512 | GLU  | 6              |
| 1   | A     | 501 | GLU  | 6              |
| 1   | A     | 462 | THR  | 5              |
| 1   | A     | 524 | LEU  | 5              |
| 1   | A     | 491 | THR  | 5              |
| 1   | A     | 518 | CYS  | 4              |
| 1   | A     | 484 | VAL  | 4              |
| 1   | A     | 472 | ARG  | 4              |
| 1   | A     | 527 | ASP  | 4              |
| 1   | A     | 459 | ILE  | 3              |
| 1   | A     | 485 | ASP  | 3              |
| 1   | A     | 490 | ASP  | 3              |
| 1   | A     | 534 | GLN  | 3              |
| 1   | A     | 511 | THR  | 2              |
| 1   | A     | 481 | VAL  | 2              |
| 1   | A     | 461 | SER  | 1              |
| 1   | A     | 523 | ILE  | 1              |
| 1   | A     | 470 | GLN  | 1              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 539 | ASP  | 1              |
| 1   | A     | 458 | LYS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 85% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `cs-full_noA.txt`

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1514 |
| Number of shifts mapped to atoms        | 1514 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 119      | $-0.55 \pm 0.07$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 113      | $-0.18 \pm 0.10$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 106      | $0.10 \pm 0.13$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 113      | $-0.28 \pm 0.31$                | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1115 atoms were assigned a chemical shift out of a possible 1228. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 419/427 (98%) | 172/172 (100%) | 164/172 (95%)   | 83/83 (100%)    |
| Sidechain | 633/716 (88%) | 435/464 (94%)  | 194/224 (87%)   | 4/28 (14%)      |

*Continued on next page...*

Continued from previous page...

|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 63/85 (74%)     | 35/41 (85%)    | 27/36 (75%)     | 1/8 (12%)       |
| Overall  | 1115/1228 (91%) | 642/677 (95%)  | 385/432 (89%)   | 88/119 (74%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1514 atoms were assigned a chemical shift out of a possible 1773. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 576/621 (93%)   | 238/251 (95%)  | 225/250 (90%)   | 113/120 (94%)   |
| Sidechain | 864/1009 (86%)  | 592/652 (91%)  | 265/313 (85%)   | 7/44 (16%)      |
| Aromatic  | 74/143 (52%)    | 42/70 (60%)    | 31/53 (58%)     | 1/20 (5%)       |
| Overall   | 1514/1773 (85%) | 872/973 (90%)  | 521/616 (85%)   | 121/184 (66%)   |

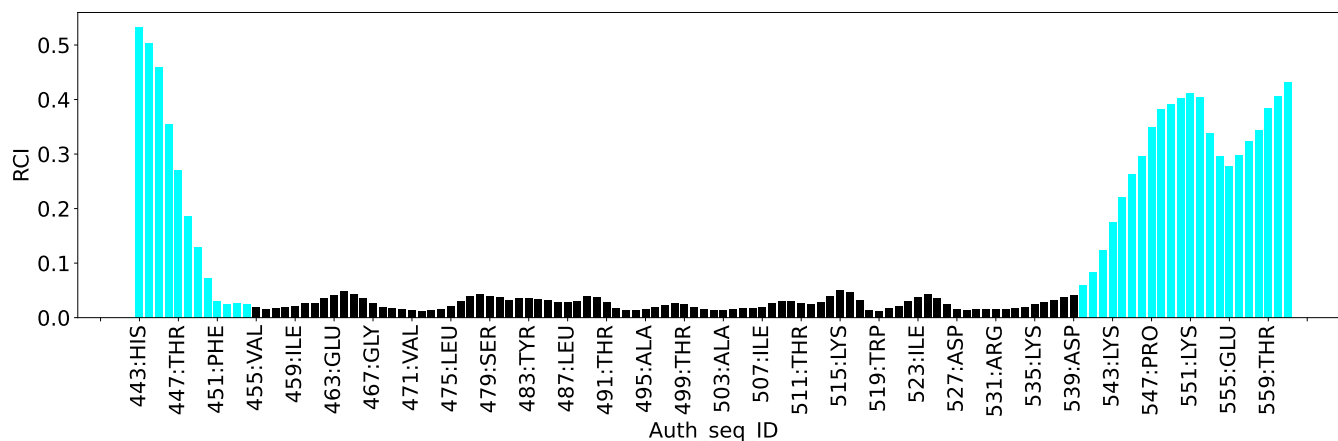
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 1253  |
| Intra-residue ( $ i-j =0$ )                              | 285   |
| Sequential ( $ i-j =1$ )                                 | 370   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 224   |
| Long range ( $ i-j \geq 5$ )                             | 286   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 88    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 135   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 11.1  |
| Number of long range restraints per residue <sup>1</sup> | 2.5   |

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 20.6                                   | 0.2     |
| 0.2-0.5 (Medium) | 35.9                                   | 0.5     |
| >0.5 (Large)     | 34.6                                   | 1.89    |

### 8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 12.1                                   | 9.96    |
| 10.0-20.0 (Medium) | 7.6                                    | 19.97   |
| >20.0 (Large)      | 73.7                                   | 170.14  |

## 9 Distance violation analysis ⓘ

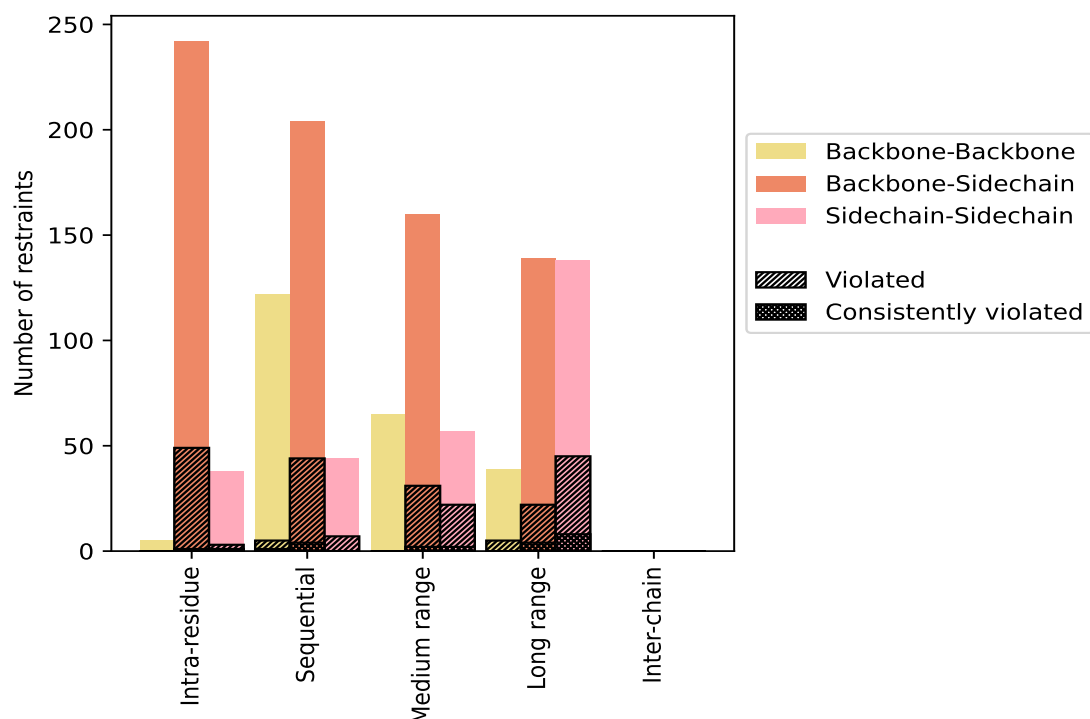
### 9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>285</b>  | <b>22.7</b>    | <b>52</b>             | <b>18.2</b>    | <b>4.2</b>     | <b>2</b>                           | <b>0.7</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 5           | 0.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 242         | 19.3           | 49                    | 20.2           | 3.9            | 1                                  | 0.4            | 0.1            |
| Sidechain-Sidechain                                                         | 38          | 3.0            | 3                     | 7.9            | 0.2            | 1                                  | 2.6            | 0.1            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>370</b>  | <b>29.5</b>    | <b>56</b>             | <b>15.1</b>    | <b>4.5</b>     | <b>5</b>                           | <b>1.4</b>     | <b>0.4</b>     |
| Backbone-Backbone                                                           | 122         | 9.7            | 5                     | 4.1            | 0.4            | 1                                  | 0.8            | 0.1            |
| Backbone-Sidechain                                                          | 204         | 16.3           | 44                    | 21.6           | 3.5            | 4                                  | 2.0            | 0.3            |
| Sidechain-Sidechain                                                         | 44          | 3.5            | 7                     | 15.9           | 0.6            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>224</b>  | <b>17.9</b>    | <b>41</b>             | <b>18.3</b>    | <b>3.3</b>     | <b>4</b>                           | <b>1.8</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 65          | 5.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 102         | 8.1            | 19                    | 18.6           | 1.5            | 2                                  | 2.0            | 0.2            |
| Sidechain-Sidechain                                                         | 57          | 4.5            | 22                    | 38.6           | 1.8            | 2                                  | 3.5            | 0.2            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>286</b>  | <b>22.8</b>    | <b>72</b>             | <b>25.2</b>    | <b>5.7</b>     | <b>12</b>                          | <b>4.2</b>     | <b>1.0</b>     |
| Backbone-Backbone                                                           | 39          | 3.1            | 5                     | 12.8           | 0.4            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 109         | 8.7            | 22                    | 20.2           | 1.8            | 4                                  | 3.7            | 0.3            |
| Sidechain-Sidechain                                                         | 138         | 11.0           | 45                    | 32.6           | 3.6            | 8                                  | 5.8            | 0.6            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>88</b>   | <b>7.0</b>     | <b>12</b>             | <b>13.6</b>    | <b>1.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>1253</b> | <b>100.0</b>   | <b>233</b>            | <b>18.6</b>    | <b>18.6</b>    | <b>23</b>                          | <b>1.8</b>     | <b>1.8</b>     |
| Backbone-Backbone                                                           | 231         | 18.4           | 10                    | 4.3            | 0.8            | 1                                  | 0.4            | 0.1            |
| Backbone-Sidechain                                                          | 745         | 59.5           | 146                   | 19.6           | 11.7           | 11                                 | 1.5            | 0.9            |
| Sidechain-Sidechain                                                         | 277         | 22.1           | 77                    | 27.8           | 6.1            | 11                                 | 4.0            | 0.9            |

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

### 9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfide bonds are counted in their appropriate category on the x-axis

## 9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 21                   | 18              | 12              | 41              | 0               | 92    | 0.48     | 1.73    | 0.33                | 0.4        |
| 2        | 16                   | 19              | 15              | 34              | 0               | 84    | 0.46     | 1.29    | 0.31                | 0.37       |
| 3        | 15                   | 26              | 17              | 37              | 0               | 95    | 0.5      | 1.74    | 0.33                | 0.42       |
| 4        | 17                   | 18              | 19              | 32              | 0               | 86    | 0.52     | 1.89    | 0.38                | 0.4        |
| 5        | 19                   | 19              | 22              | 37              | 0               | 97    | 0.54     | 1.83    | 0.39                | 0.44       |
| 6        | 20                   | 16              | 19              | 32              | 0               | 87    | 0.5      | 1.83    | 0.35                | 0.39       |
| 7        | 15                   | 24              | 17              | 41              | 0               | 97    | 0.46     | 1.87    | 0.36                | 0.37       |
| 8        | 22                   | 15              | 17              | 37              | 0               | 91    | 0.5      | 1.64    | 0.35                | 0.38       |
| 9        | 20                   | 15              | 17              | 35              | 0               | 87    | 0.53     | 1.74    | 0.36                | 0.47       |
| 10       | 17                   | 19              | 15              | 39              | 0               | 90    | 0.51     | 1.7     | 0.37                | 0.42       |

*Continued on next page...*

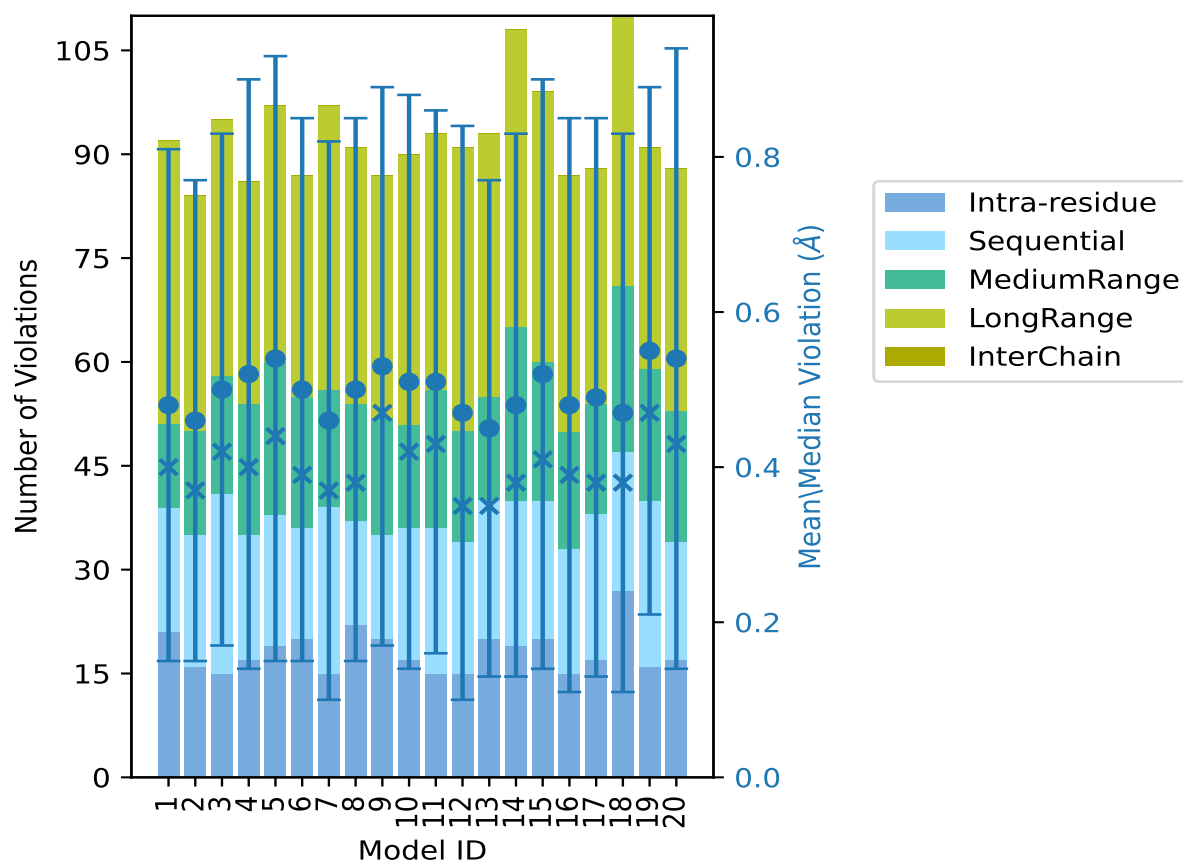
Continued from previous page...

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 15                   | 21              | 20              | 37              | 0               | 93    | 0.51     | 1.69    | 0.35                | 0.43       |
| 12       | 15                   | 19              | 16              | 41              | 0               | 91    | 0.47     | 1.86    | 0.37                | 0.35       |
| 13       | 20                   | 20              | 15              | 38              | 0               | 93    | 0.45     | 1.61    | 0.32                | 0.35       |
| 14       | 19                   | 21              | 25              | 43              | 0               | 108   | 0.48     | 1.82    | 0.35                | 0.38       |
| 15       | 20                   | 20              | 20              | 39              | 0               | 99    | 0.52     | 1.6     | 0.38                | 0.41       |
| 16       | 15                   | 18              | 17              | 37              | 0               | 87    | 0.48     | 1.65    | 0.37                | 0.39       |
| 17       | 17                   | 21              | 16              | 34              | 0               | 88    | 0.49     | 1.84    | 0.36                | 0.38       |
| 18       | 27                   | 20              | 24              | 39              | 0               | 110   | 0.47     | 1.84    | 0.36                | 0.38       |
| 19       | 16                   | 24              | 19              | 32              | 0               | 91    | 0.55     | 1.59    | 0.34                | 0.47       |
| 20       | 17                   | 17              | 19              | 35              | 0               | 88    | 0.54     | 1.84    | 0.4                 | 0.43       |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

### 9.3 Distance violation statistics for the ensemble

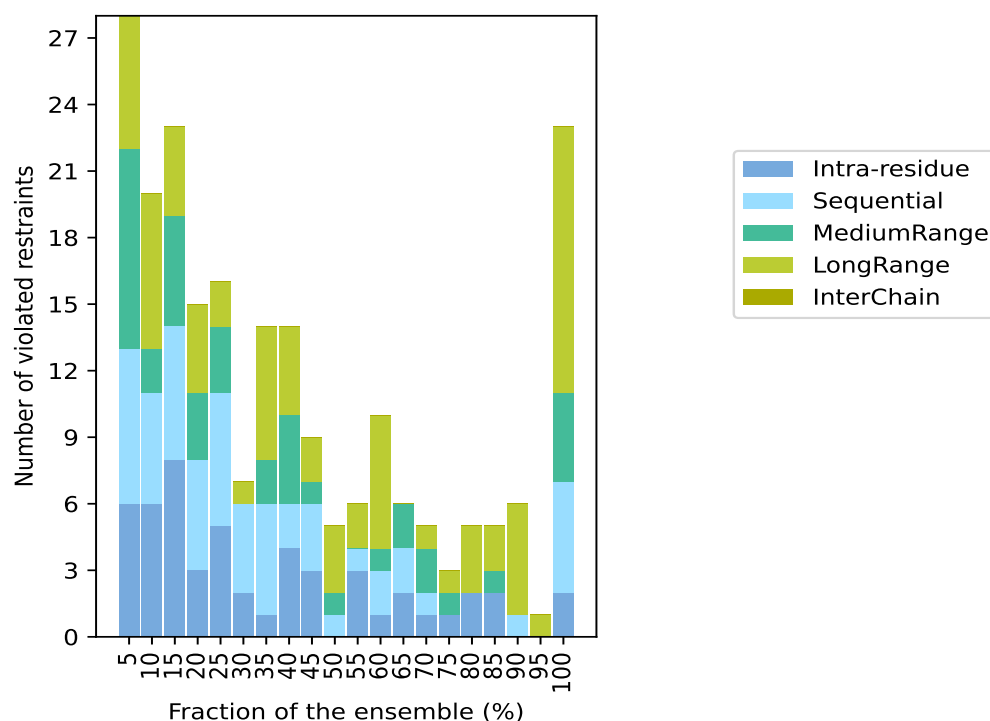
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 944(IR:233, SQ:314, MR:183, LR:214, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 6                             | 7               | 9               | 6               | 0               | 28    | 1                        | 5.0   |
| 6                             | 5               | 2               | 7               | 0               | 20    | 2                        | 10.0  |
| 8                             | 6               | 5               | 4               | 0               | 23    | 3                        | 15.0  |
| 3                             | 5               | 3               | 4               | 0               | 15    | 4                        | 20.0  |
| 5                             | 6               | 3               | 2               | 0               | 16    | 5                        | 25.0  |
| 2                             | 4               | 0               | 1               | 0               | 7     | 6                        | 30.0  |
| 1                             | 5               | 2               | 6               | 0               | 14    | 7                        | 35.0  |
| 4                             | 2               | 4               | 4               | 0               | 14    | 8                        | 40.0  |
| 3                             | 3               | 1               | 2               | 0               | 9     | 9                        | 45.0  |
| 0                             | 1               | 1               | 3               | 0               | 5     | 10                       | 50.0  |
| 3                             | 1               | 0               | 2               | 0               | 6     | 11                       | 55.0  |
| 1                             | 2               | 1               | 6               | 0               | 10    | 12                       | 60.0  |
| 2                             | 2               | 2               | 0               | 0               | 6     | 13                       | 65.0  |
| 1                             | 1               | 2               | 1               | 0               | 5     | 14                       | 70.0  |
| 1                             | 0               | 1               | 1               | 0               | 3     | 15                       | 75.0  |
| 2                             | 0               | 0               | 3               | 0               | 5     | 16                       | 80.0  |
| 2                             | 0               | 1               | 2               | 0               | 5     | 17                       | 85.0  |
| 0                             | 1               | 0               | 5               | 0               | 6     | 18                       | 90.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 19                       | 95.0  |
| 2                             | 5               | 4               | 12              | 0               | 23    | 20                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

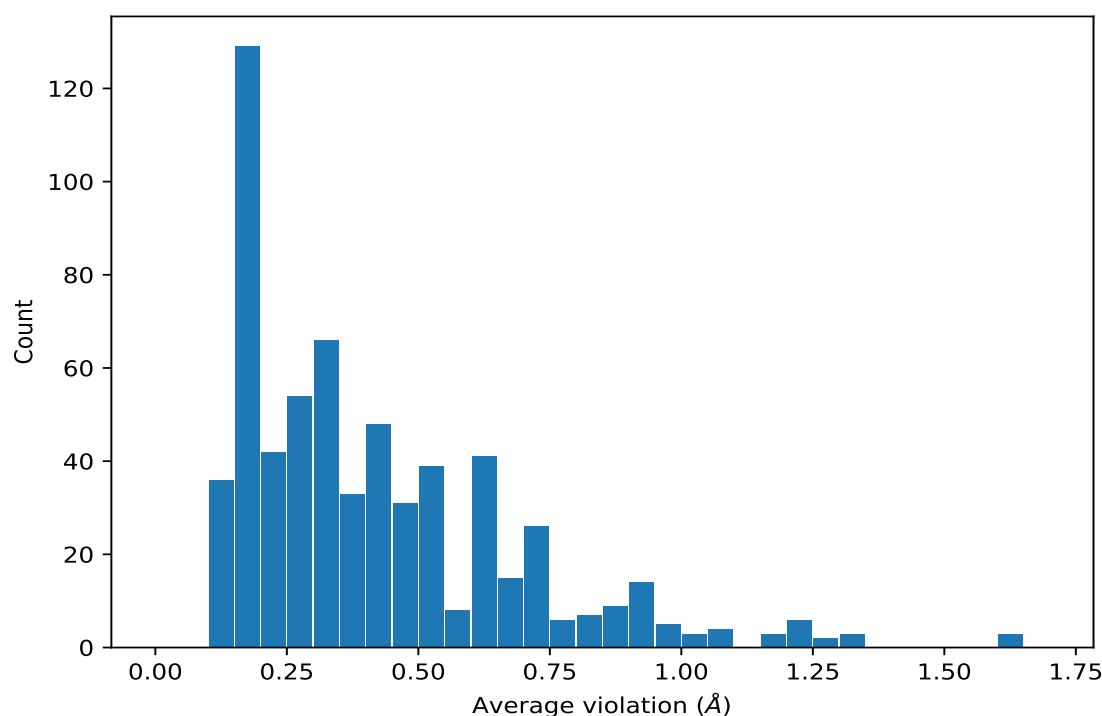
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 9.4 Most violated distance restraints in the ensemble [i](#)

### 9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



#### 9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA   | 20                  | 1.61     | 0.19                | 1.67       |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 20                  | 1.34     | 0.11                | 1.31       |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 20                  | 1.34     | 0.11                | 1.31       |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 20                  | 1.34     | 0.11                | 1.31       |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 20                  | 1.26     | 0.03                | 1.27       |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 20                  | 1.26     | 0.03                | 1.27       |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 20                  | 1.18     | 0.11                | 1.17       |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 20                  | 1.0      | 0.23                | 0.94       |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 20                  | 0.97     | 0.05                | 0.98       |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 20                  | 0.94     | 0.23                | 0.91       |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 20                  | 0.94     | 0.23                | 0.91       |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 20                  | 0.85     | 0.11                | 0.86       |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 20                  | 0.85     | 0.11                | 0.86       |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 20                  | 0.79     | 0.23                | 0.86       |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 20                  | 0.74     | 0.13                | 0.68       |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 20                  | 0.74     | 0.13                | 0.68       |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 20                  | 0.74     | 0.13                | 0.68       |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 20                  | 0.74     | 0.13                | 0.68       |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 20                  | 0.74     | 0.13                | 0.68       |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 20                  | 0.74     | 0.13                | 0.68       |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 20                  | 0.72     | 0.43                | 0.55       |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 20                  | 0.72     | 0.43                | 0.55       |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 20                  | 0.72     | 0.43                | 0.55       |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 20                  | 0.72     | 0.43                | 0.55       |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 20                  | 0.69     | 0.08                | 0.68       |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 20                  | 0.65     | 0.05                | 0.63       |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 20                  | 0.65     | 0.05                | 0.63       |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 20                  | 0.65     | 0.05                | 0.63       |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 20                  | 0.65     | 0.05                | 0.63       |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 20                  | 0.65     | 0.05                | 0.63       |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 20                  | 0.65     | 0.05                | 0.63       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 20                  | 0.61     | 0.26                | 0.68       |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 20                  | 0.58     | 0.12                | 0.57       |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 20                  | 0.48     | 0.16                | 0.46       |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 20                  | 0.48     | 0.16                | 0.46       |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 20                  | 0.48     | 0.03                | 0.48       |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 20                  | 0.48     | 0.03                | 0.48       |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 20                  | 0.44     | 0.1                 | 0.45       |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 20                  | 0.44     | 0.1                 | 0.45       |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 20                  | 0.42     | 0.08                | 0.42       |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 20                  | 0.41     | 0.07                | 0.44       |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 20                  | 0.41     | 0.07                | 0.44       |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 20                  | 0.39     | 0.03                | 0.4        |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 20                  | 0.39     | 0.03                | 0.4        |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 20                  | 0.39     | 0.03                | 0.4        |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 20                  | 0.38     | 0.02                | 0.38       |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 20                  | 0.32     | 0.13                | 0.28       |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 19                  | 0.48     | 0.1                 | 0.49       |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 18                  | 1.2      | 0.44                | 1.0        |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 18                  | 1.2      | 0.44                | 1.0        |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 18                  | 1.2      | 0.44                | 1.0        |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 18                  | 1.2      | 0.44                | 1.0        |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 18                  | 1.2      | 0.44                | 1.0        |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 18                  | 1.2      | 0.44                | 1.0        |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 18                  | 0.62     | 0.19                | 0.6        |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 18                  | 0.62     | 0.19                | 0.6        |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 18                  | 0.54     | 0.24                | 0.52       |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 18                  | 0.54     | 0.24                | 0.52       |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 18                  | 0.5      | 0.25                | 0.46       |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 18                  | 0.5      | 0.25                | 0.46       |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 18                  | 0.5      | 0.25                | 0.46       |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 18                  | 0.5      | 0.25                | 0.46       |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 18                  | 0.5      | 0.25                | 0.46       |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 18                  | 0.5      | 0.25                | 0.46       |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 18                  | 0.39     | 0.13                | 0.43       |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 18                  | 0.26     | 0.1                 | 0.26       |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 17                  | 0.62     | 0.29                | 0.58       |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 17                  | 0.48     | 0.31                | 0.5        |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 17                  | 0.48     | 0.31                | 0.5        |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 17                  | 0.48     | 0.31                | 0.5        |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 17                  | 0.48     | 0.31                | 0.5        |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 17                  | 0.37     | 0.14                | 0.39       |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 17                  | 0.37     | 0.14                | 0.39       |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 17                  | 0.37     | 0.14                | 0.39       |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 17                  | 0.35     | 0.18                | 0.26       |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 17                  | 0.16     | 0.03                | 0.15       |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 17                  | 0.16     | 0.03                | 0.15       |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 17                  | 0.16     | 0.03                | 0.15       |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 17                  | 0.16     | 0.03                | 0.15       |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 17                  | 0.16     | 0.03                | 0.15       |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 17                  | 0.16     | 0.03                | 0.15       |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 16                  | 0.51     | 0.26                | 0.51       |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 16                  | 0.49     | 0.09                | 0.52       |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 16                  | 0.49     | 0.09                | 0.52       |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 16                  | 0.49     | 0.09                | 0.52       |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 16                  | 0.49     | 0.09                | 0.52       |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 16                  | 0.49     | 0.09                | 0.52       |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 16                  | 0.49     | 0.09                | 0.52       |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 16                  | 0.31     | 0.08                | 0.3        |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 16                  | 0.31     | 0.08                | 0.3        |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 16                  | 0.26     | 0.15                | 0.18       |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 16                  | 0.26     | 0.15                | 0.18       |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 16                  | 0.26     | 0.15                | 0.18       |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 16                  | 0.26     | 0.15                | 0.18       |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 16                  | 0.26     | 0.15                | 0.18       |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 16                  | 0.26     | 0.15                | 0.18       |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 16                  | 0.14     | 0.02                | 0.14       |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 15                  | 0.61     | 0.23                | 0.63       |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 15                  | 0.61     | 0.34                | 0.63       |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 15                  | 0.61     | 0.34                | 0.63       |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 15                  | 0.61     | 0.34                | 0.63       |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 15                  | 0.61     | 0.34                | 0.63       |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 15                  | 0.61     | 0.34                | 0.63       |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 15                  | 0.61     | 0.34                | 0.63       |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 15                  | 0.41     | 0.13                | 0.45       |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 15                  | 0.41     | 0.13                | 0.45       |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 15                  | 0.41     | 0.13                | 0.45       |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 15                  | 0.41     | 0.13                | 0.45       |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 15                  | 0.41     | 0.13                | 0.45       |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 15                  | 0.41     | 0.13                | 0.45       |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 14                  | 0.77     | 0.19                | 0.8        |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 14                  | 0.77     | 0.19                | 0.8        |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 14                  | 0.41     | 0.13                | 0.45       |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 14                  | 0.41     | 0.13                | 0.45       |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 14                  | 0.33     | 0.12                | 0.34       |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 14                  | 0.33     | 0.12                | 0.34       |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 14                  | 0.28     | 0.09                | 0.29       |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 14                  | 0.28     | 0.09                | 0.29       |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD2  | 14                  | 0.16     | 0.01                | 0.16       |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD3  | 14                  | 0.16     | 0.01                | 0.16       |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 13                  | 0.88     | 0.28                | 0.95       |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 13                  | 0.88     | 0.28                | 0.95       |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2  | 13                  | 0.85     | 0.38                | 0.79       |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 13                  | 0.85     | 0.38                | 0.79       |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 13                  | 0.75     | 0.45                | 0.86       |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 13                  | 0.46     | 0.27                | 0.35       |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 13                  | 0.46     | 0.27                | 0.35       |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 13                  | 0.27     | 0.15                | 0.21       |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 13                  | 0.27     | 0.15                | 0.21       |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 13                  | 0.18     | 0.05                | 0.18       |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 13                  | 0.18     | 0.05                | 0.18       |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 13                  | 0.18     | 0.05                | 0.18       |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 13                  | 0.18     | 0.05                | 0.18       |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 13                  | 0.18     | 0.05                | 0.18       |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 13                  | 0.18     | 0.05                | 0.18       |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 12                  | 0.74     | 0.25                | 0.8        |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 12                  | 0.55     | 0.07                | 0.56       |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 12                  | 0.55     | 0.07                | 0.56       |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |

*Continued on next page...*

Continued from previous page...

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 12                  | 0.44     | 0.27                | 0.36       |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 12                  | 0.42     | 0.13                | 0.39       |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 12                  | 0.42     | 0.13                | 0.39       |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 12                  | 0.42     | 0.13                | 0.39       |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 12                  | 0.42     | 0.13                | 0.39       |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 12                  | 0.41     | 0.17                | 0.41       |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 12                  | 0.41     | 0.17                | 0.41       |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 12                  | 0.41     | 0.17                | 0.41       |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 12                  | 0.41     | 0.17                | 0.41       |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 12                  | 0.35     | 0.14                | 0.31       |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 12                  | 0.35     | 0.14                | 0.31       |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 12                  | 0.35     | 0.09                | 0.39       |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 12                  | 0.35     | 0.09                | 0.39       |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 12                  | 0.31     | 0.12                | 0.27       |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 12                  | 0.31     | 0.12                | 0.27       |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 12                  | 0.31     | 0.12                | 0.27       |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 12                  | 0.31     | 0.12                | 0.27       |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 12                  | 0.31     | 0.12                | 0.27       |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 12                  | 0.31     | 0.12                | 0.27       |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 12                  | 0.28     | 0.05                | 0.28       |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 12                  | 0.28     | 0.05                | 0.28       |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 12                  | 0.23     | 0.07                | 0.27       |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 12                  | 0.23     | 0.07                | 0.27       |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 12                  | 0.23     | 0.07                | 0.27       |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 11                  | 0.51     | 0.23                | 0.51       |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 11                  | 0.51     | 0.23                | 0.51       |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 11                  | 0.51     | 0.23                | 0.51       |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 11                  | 0.51     | 0.23                | 0.51       |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 11                  | 0.51     | 0.22                | 0.48       |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 11                  | 0.51     | 0.22                | 0.48       |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2  | 11                  | 0.36     | 0.17                | 0.38       |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2  | 11                  | 0.36     | 0.17                | 0.38       |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB2  | 11                  | 0.22     | 0.07                | 0.21       |

Continued on next page...

*Continued from previous page...*

| Key     | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (3,201) | 1:482:A:LEU:HB2 | 1:483:A:TYR:HB3  | 11                  | 0.22     | 0.07                | 0.21       |
| (3,201) | 1:482:A:LEU:HB3 | 1:483:A:TYR:HB2  | 11                  | 0.22     | 0.07                | 0.21       |
| (3,201) | 1:482:A:LEU:HB3 | 1:483:A:TYR:HB3  | 11                  | 0.22     | 0.07                | 0.21       |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD11 | 11                  | 0.19     | 0.08                | 0.16       |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD12 | 11                  | 0.19     | 0.08                | 0.16       |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD13 | 11                  | 0.19     | 0.08                | 0.16       |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD21 | 11                  | 0.19     | 0.08                | 0.16       |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD22 | 11                  | 0.19     | 0.08                | 0.16       |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD23 | 11                  | 0.19     | 0.08                | 0.16       |
| (3,522) | 1:516:A:LYS:HA  | 1:516:A:LYS:HE2  | 11                  | 0.16     | 0.02                | 0.15       |
| (3,522) | 1:516:A:LYS:HA  | 1:516:A:LYS:HE3  | 11                  | 0.16     | 0.02                | 0.15       |
| (3,233) | 1:486:A:LEU:HG  | 1:487:A:LEU:H    | 10                  | 0.37     | 0.1                 | 0.38       |
| (3,30)  | 1:451:A:PHE:HE1 | 1:453:A:SER:HB2  | 10                  | 0.32     | 0.15                | 0.3        |
| (3,30)  | 1:451:A:PHE:HE2 | 1:453:A:SER:HB2  | 10                  | 0.32     | 0.15                | 0.3        |
| (3,30)  | 1:451:A:PHE:HE1 | 1:453:A:SER:HB3  | 10                  | 0.32     | 0.15                | 0.3        |
| (3,30)  | 1:451:A:PHE:HE2 | 1:453:A:SER:HB3  | 10                  | 0.32     | 0.15                | 0.3        |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD11 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD12 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD13 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD21 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD22 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD23 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD11 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD12 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD13 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD21 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD22 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,618) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HD23 | 10                  | 0.29     | 0.08                | 0.29       |
| (3,401) | 1:497:A:PHE:HD1 | 1:502:A:ASP:HB2  | 10                  | 0.26     | 0.12                | 0.28       |
| (3,401) | 1:497:A:PHE:HD1 | 1:502:A:ASP:HB3  | 10                  | 0.26     | 0.12                | 0.28       |
| (3,401) | 1:497:A:PHE:HD2 | 1:502:A:ASP:HB2  | 10                  | 0.26     | 0.12                | 0.28       |
| (3,401) | 1:497:A:PHE:HD2 | 1:502:A:ASP:HB3  | 10                  | 0.26     | 0.12                | 0.28       |
| (3,325) | 1:485:A:ASP:H   | 1:495:A:ALA:HA   | 10                  | 0.2      | 0.06                | 0.21       |
| (1,13)  | 1:474:A:THR:O   | 1:478:A:ILE:H    | 10                  | 0.13     | 0.01                | 0.13       |
| (3,617) | 1:510:A:TYR:HB2 | 1:521:A:LEU:HG   | 9                   | 0.81     | 0.18                | 0.83       |
| (3,914) | 1:559:A:THR:H   | 1:559:A:THR:HG21 | 9                   | 0.8      | 0.37                | 0.88       |
| (3,914) | 1:559:A:THR:H   | 1:559:A:THR:HG22 | 9                   | 0.8      | 0.37                | 0.88       |
| (3,914) | 1:559:A:THR:H   | 1:559:A:THR:HG23 | 9                   | 0.8      | 0.37                | 0.88       |
| (3,872) | 1:545:A:ASN:H   | 1:545:A:ASN:HD21 | 9                   | 0.72     | 0.48                | 0.74       |
| (3,872) | 1:545:A:ASN:H   | 1:545:A:ASN:HD22 | 9                   | 0.72     | 0.48                | 0.74       |
| (3,886) | 1:549:A:GLU:H   | 1:549:A:GLU:HG2  | 9                   | 0.71     | 0.29                | 0.66       |
| (3,886) | 1:549:A:GLU:H   | 1:549:A:GLU:HG3  | 9                   | 0.71     | 0.29                | 0.66       |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,913) | 1:558:A:ILE:HG21 | 1:559:A:THR:H    | 9                   | 0.69     | 0.37                | 0.62       |
| (3,913) | 1:558:A:ILE:HG22 | 1:559:A:THR:H    | 9                   | 0.69     | 0.37                | 0.62       |
| (3,913) | 1:558:A:ILE:HG23 | 1:559:A:THR:H    | 9                   | 0.69     | 0.37                | 0.62       |
| (3,29)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HA   | 9                   | 0.46     | 0.16                | 0.42       |
| (3,29)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HA   | 9                   | 0.46     | 0.16                | 0.42       |
| (3,725) | 1:531:A:ARG:HD2  | 1:532:A:TYR:H    | 9                   | 0.34     | 0.19                | 0.28       |
| (3,725) | 1:531:A:ARG:HD3  | 1:532:A:TYR:H    | 9                   | 0.34     | 0.19                | 0.28       |
| (3,303) | 1:459:A:ILE:HG12 | 1:494:A:HIS:HA   | 9                   | 0.27     | 0.11                | 0.26       |
| (3,303) | 1:459:A:ILE:HG13 | 1:494:A:HIS:HA   | 9                   | 0.27     | 0.11                | 0.26       |
| (1,35)  | 1:500:A:PRO:O    | 1:504:A:GLN:H    | 9                   | 0.26     | 0.15                | 0.21       |
| (3,410) | 1:501:A:GLU:HG2  | 1:502:A:ASP:H    | 9                   | 0.24     | 0.08                | 0.28       |
| (3,410) | 1:501:A:GLU:HG3  | 1:502:A:ASP:H    | 9                   | 0.24     | 0.08                | 0.28       |
| (1,43)  | 1:504:A:GLN:O    | 1:508:A:ASN:H    | 9                   | 0.19     | 0.05                | 0.17       |
| (1,71)  | 1:531:A:ARG:O    | 1:535:A:LYS:H    | 9                   | 0.12     | 0.03                | 0.12       |
| (3,1)   | 1:445:A:ASN:HB2  | 1:446:A:ALA:H    | 8                   | 1.08     | 0.37                | 1.15       |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 8                   | 0.94     | 0.13                | 0.95       |
| (3,619) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HG   | 8                   | 0.82     | 0.26                | 0.82       |
| (3,874) | 1:545:A:ASN:H    | 1:546:A:GLN:H    | 8                   | 0.62     | 0.46                | 0.44       |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG21 | 8                   | 0.52     | 0.19                | 0.57       |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG22 | 8                   | 0.52     | 0.19                | 0.57       |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG23 | 8                   | 0.52     | 0.19                | 0.57       |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD11 | 8                   | 0.44     | 0.14                | 0.46       |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD12 | 8                   | 0.44     | 0.14                | 0.46       |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD13 | 8                   | 0.44     | 0.14                | 0.46       |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD21 | 8                   | 0.44     | 0.14                | 0.46       |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD22 | 8                   | 0.44     | 0.14                | 0.46       |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD23 | 8                   | 0.44     | 0.14                | 0.46       |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE21 | 8                   | 0.39     | 0.23                | 0.36       |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE22 | 8                   | 0.39     | 0.23                | 0.36       |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB2  | 8                   | 0.37     | 0.14                | 0.36       |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB3  | 8                   | 0.37     | 0.14                | 0.36       |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG2  | 8                   | 0.34     | 0.11                | 0.36       |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG3  | 8                   | 0.34     | 0.11                | 0.36       |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG2  | 8                   | 0.34     | 0.11                | 0.36       |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG3  | 8                   | 0.34     | 0.11                | 0.36       |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD2  | 8                   | 0.26     | 0.1                 | 0.24       |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD2  | 8                   | 0.26     | 0.1                 | 0.24       |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD2  | 8                   | 0.26     | 0.1                 | 0.24       |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD3  | 8                   | 0.26     | 0.1                 | 0.24       |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD3  | 8                   | 0.26     | 0.1                 | 0.24       |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD3  | 8                   | 0.26     | 0.1                 | 0.24       |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB1  | 8                   | 0.21     | 0.09                | 0.17       |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB2  | 8                   | 0.21     | 0.09                | 0.17       |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB3  | 8                   | 0.21     | 0.09                | 0.17       |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE1  | 8                   | 0.2      | 0.09                | 0.18       |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE2  | 8                   | 0.2      | 0.09                | 0.18       |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG21 | 8                   | 0.2      | 0.08                | 0.18       |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG22 | 8                   | 0.2      | 0.08                | 0.18       |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG23 | 8                   | 0.2      | 0.08                | 0.18       |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE2  | 8                   | 0.16     | 0.04                | 0.15       |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE3  | 8                   | 0.16     | 0.04                | 0.15       |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE2  | 8                   | 0.16     | 0.04                | 0.15       |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE3  | 8                   | 0.16     | 0.04                | 0.15       |
| (3,900) | 1:554:A:THR:HG21 | 1:555:A:GLU:H    | 7                   | 1.09     | 0.49                | 1.11       |
| (3,900) | 1:554:A:THR:HG22 | 1:555:A:GLU:H    | 7                   | 1.09     | 0.49                | 1.11       |
| (3,900) | 1:554:A:THR:HG23 | 1:555:A:GLU:H    | 7                   | 1.09     | 0.49                | 1.11       |
| (3,899) | 1:554:A:THR:H    | 1:555:A:GLU:H    | 7                   | 0.86     | 0.34                | 0.97       |
| (3,436) | 1:479:A:SER:HB2  | 1:506:A:VAL:HB   | 7                   | 0.76     | 0.32                | 0.78       |
| (3,436) | 1:479:A:SER:HB3  | 1:506:A:VAL:HB   | 7                   | 0.76     | 0.32                | 0.78       |
| (3,911) | 1:558:A:ILE:HB   | 1:559:A:THR:H    | 7                   | 0.56     | 0.29                | 0.55       |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD2  | 7                   | 0.48     | 0.21                | 0.49       |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD3  | 7                   | 0.48     | 0.21                | 0.49       |
| (3,731) | 1:451:A:PHE:HD1  | 1:533:A:TRP:HB3  | 7                   | 0.35     | 0.26                | 0.29       |
| (3,731) | 1:451:A:PHE:HD2  | 1:533:A:TRP:HB3  | 7                   | 0.35     | 0.26                | 0.29       |
| (3,746) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HZ2  | 7                   | 0.33     | 0.19                | 0.26       |
| (3,746) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HZ2  | 7                   | 0.33     | 0.19                | 0.26       |
| (3,6)   | 1:446:A:ALA:HB1  | 1:447:A:THR:H    | 7                   | 0.32     | 0.12                | 0.35       |
| (3,6)   | 1:446:A:ALA:HB2  | 1:447:A:THR:H    | 7                   | 0.32     | 0.12                | 0.35       |
| (3,6)   | 1:446:A:ALA:HB3  | 1:447:A:THR:H    | 7                   | 0.32     | 0.12                | 0.35       |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD11 | 7                   | 0.25     | 0.08                | 0.24       |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD12 | 7                   | 0.25     | 0.08                | 0.24       |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD13 | 7                   | 0.25     | 0.08                | 0.24       |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG21 | 7                   | 0.24     | 0.13                | 0.19       |

*Continued on next page...*

Continued from previous page...

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG22 | 7                   | 0.24     | 0.13                | 0.19       |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG23 | 7                   | 0.24     | 0.13                | 0.19       |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB2  | 7                   | 0.19     | 0.03                | 0.19       |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB3  | 7                   | 0.19     | 0.03                | 0.19       |
| (3,694) | 1:451:A:PHE:HZ   | 1:530:A:GLN:HA   | 7                   | 0.16     | 0.05                | 0.15       |
| (3,112) | 1:468:A:ARG:HG2  | 1:469:A:LYS:H    | 7                   | 0.13     | 0.03                | 0.13       |
| (3,112) | 1:468:A:ARG:HG3  | 1:469:A:LYS:H    | 7                   | 0.13     | 0.03                | 0.13       |
| (3,585) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HE1  | 7                   | 0.12     | 0.02                | 0.12       |
| (3,585) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HE1  | 7                   | 0.12     | 0.02                | 0.12       |
| (3,585) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HE1  | 7                   | 0.12     | 0.02                | 0.12       |
| (3,896) | 1:553:A:GLY:H    | 1:554:A:THR:H    | 6                   | 0.64     | 0.32                | 0.6        |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG2  | 6                   | 0.5      | 0.37                | 0.38       |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG3  | 6                   | 0.5      | 0.37                | 0.38       |
| (3,895) | 1:552:A:ARG:HB2  | 1:553:A:GLY:H    | 6                   | 0.47     | 0.25                | 0.52       |
| (3,895) | 1:552:A:ARG:HB3  | 1:553:A:GLY:H    | 6                   | 0.47     | 0.25                | 0.52       |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD11 | 6                   | 0.32     | 0.04                | 0.32       |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD12 | 6                   | 0.32     | 0.04                | 0.32       |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD13 | 6                   | 0.32     | 0.04                | 0.32       |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD21 | 6                   | 0.32     | 0.04                | 0.32       |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD22 | 6                   | 0.32     | 0.04                | 0.32       |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD23 | 6                   | 0.32     | 0.04                | 0.32       |
| (1,39)  | 1:502:A:ASP:O    | 1:506:A:VAL:H    | 6                   | 0.27     | 0.08                | 0.29       |
| (3,706) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 6                   | 0.26     | 0.08                | 0.26       |
| (3,706) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 6                   | 0.26     | 0.08                | 0.26       |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD21 | 6                   | 0.21     | 0.06                | 0.22       |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD21 | 6                   | 0.21     | 0.06                | 0.22       |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD22 | 6                   | 0.21     | 0.06                | 0.22       |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD22 | 6                   | 0.21     | 0.06                | 0.22       |
| (3,412) | 1:455:A:VAL:HG11 | 1:503:A:ALA:H    | 6                   | 0.16     | 0.05                | 0.13       |
| (3,412) | 1:455:A:VAL:HG12 | 1:503:A:ALA:H    | 6                   | 0.16     | 0.05                | 0.13       |
| (3,412) | 1:455:A:VAL:HG13 | 1:503:A:ALA:H    | 6                   | 0.16     | 0.05                | 0.13       |
| (3,412) | 1:455:A:VAL:HG21 | 1:503:A:ALA:H    | 6                   | 0.16     | 0.05                | 0.13       |
| (3,412) | 1:455:A:VAL:HG22 | 1:503:A:ALA:H    | 6                   | 0.16     | 0.05                | 0.13       |
| (3,412) | 1:455:A:VAL:HG23 | 1:503:A:ALA:H    | 6                   | 0.16     | 0.05                | 0.13       |
| (3,889) | 1:549:A:GLU:HG2  | 1:550:A:LYS:H    | 5                   | 0.85     | 0.32                | 0.89       |
| (3,889) | 1:549:A:GLU:HG3  | 1:550:A:LYS:H    | 5                   | 0.85     | 0.32                | 0.89       |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD2  | 5                   | 0.8      | 0.4                 | 0.92       |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD3  | 5                   | 0.8      | 0.4                 | 0.92       |
| (3,39)  | 1:455:A:VAL:H    | 1:456:A:ILE:H    | 5                   | 0.58     | 0.03                | 0.57       |
| (3,863) | 1:541:A:GLN:HA   | 1:541:A:GLN:HE21 | 5                   | 0.48     | 0.36                | 0.37       |
| (3,863) | 1:541:A:GLN:HA   | 1:541:A:GLN:HE22 | 5                   | 0.48     | 0.36                | 0.37       |
| (3,355) | 1:455:A:VAL:HG11 | 1:497:A:PHE:H    | 5                   | 0.47     | 0.07                | 0.46       |

Continued on next page...

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,355) | 1:455:A:VAL:HG12 | 1:497:A:PHE:H    | 5                   | 0.47     | 0.07                | 0.46       |
| (3,355) | 1:455:A:VAL:HG13 | 1:497:A:PHE:H    | 5                   | 0.47     | 0.07                | 0.46       |
| (3,355) | 1:455:A:VAL:HG21 | 1:497:A:PHE:H    | 5                   | 0.47     | 0.07                | 0.46       |
| (3,355) | 1:455:A:VAL:HG22 | 1:497:A:PHE:H    | 5                   | 0.47     | 0.07                | 0.46       |
| (3,355) | 1:455:A:VAL:HG23 | 1:497:A:PHE:H    | 5                   | 0.47     | 0.07                | 0.46       |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG2  | 5                   | 0.43     | 0.17                | 0.33       |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG3  | 5                   | 0.43     | 0.17                | 0.33       |
| (3,493) | 1:511:A:THR:HG21 | 1:512:A:GLU:H    | 5                   | 0.4      | 0.06                | 0.4        |
| (3,493) | 1:511:A:THR:HG22 | 1:512:A:GLU:H    | 5                   | 0.4      | 0.06                | 0.4        |
| (3,493) | 1:511:A:THR:HG23 | 1:512:A:GLU:H    | 5                   | 0.4      | 0.06                | 0.4        |
| (3,456) | 1:507:A:ILE:HD11 | 1:508:A:ASN:H    | 5                   | 0.35     | 0.13                | 0.39       |
| (3,456) | 1:507:A:ILE:HD12 | 1:508:A:ASN:H    | 5                   | 0.35     | 0.13                | 0.39       |
| (3,456) | 1:507:A:ILE:HD13 | 1:508:A:ASN:H    | 5                   | 0.35     | 0.13                | 0.39       |
| (1,37)  | 1:501:A:GLU:O    | 1:505:A:ALA:H    | 5                   | 0.34     | 0.14                | 0.39       |
| (3,457) | 1:507:A:ILE:HD11 | 1:508:A:ASN:HD22 | 5                   | 0.28     | 0.05                | 0.26       |
| (3,457) | 1:507:A:ILE:HD12 | 1:508:A:ASN:HD22 | 5                   | 0.28     | 0.05                | 0.26       |
| (3,457) | 1:507:A:ILE:HD13 | 1:508:A:ASN:HD22 | 5                   | 0.28     | 0.05                | 0.26       |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD2  | 5                   | 0.26     | 0.05                | 0.25       |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD3  | 5                   | 0.26     | 0.05                | 0.25       |
| (3,653) | 1:524:A:LEU:H    | 1:524:A:LEU:HG   | 5                   | 0.25     | 0.13                | 0.2        |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD11 | 5                   | 0.19     | 0.06                | 0.16       |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD12 | 5                   | 0.19     | 0.06                | 0.16       |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD13 | 5                   | 0.19     | 0.06                | 0.16       |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD11 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD12 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD13 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD21 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD22 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD23 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD11 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD12 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD13 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD21 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD22 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD23 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD11 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD12 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD13 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD21 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD22 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD23 | 5                   | 0.18     | 0.07                | 0.15       |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD11 | 5                   | 0.17     | 0.08                | 0.12       |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD12 | 5                   | 0.17     | 0.08                | 0.12       |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD13 | 5                   | 0.17     | 0.08                | 0.12       |
| (3,379) | 1:497:A:PHE:HB2  | 1:498:A:LYS:H    | 5                   | 0.14     | 0.02                | 0.14       |
| (3,379) | 1:497:A:PHE:HB3  | 1:498:A:LYS:H    | 5                   | 0.14     | 0.02                | 0.14       |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD2  | 5                   | 0.13     | 0.05                | 0.11       |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD3  | 5                   | 0.13     | 0.05                | 0.11       |
| (3,893) | 1:552:A:ARG:H    | 1:552:A:ARG:HD2  | 4                   | 1.17     | 0.5                 | 1.08       |
| (3,893) | 1:552:A:ARG:H    | 1:552:A:ARG:HD3  | 4                   | 1.17     | 0.5                 | 1.08       |
| (3,255) | 1:460:A:ILE:HD11 | 1:492:A:GLU:HA   | 4                   | 0.66     | 0.12                | 0.73       |
| (3,255) | 1:460:A:ILE:HD12 | 1:492:A:GLU:HA   | 4                   | 0.66     | 0.12                | 0.73       |
| (3,255) | 1:460:A:ILE:HD13 | 1:492:A:GLU:HA   | 4                   | 0.66     | 0.12                | 0.73       |
| (3,260) | 1:490:A:ASP:HB3  | 1:492:A:GLU:HG2  | 4                   | 0.41     | 0.08                | 0.4        |
| (3,260) | 1:490:A:ASP:HB3  | 1:492:A:GLU:HG3  | 4                   | 0.41     | 0.08                | 0.4        |
| (3,103) | 1:466:A:PRO:HD2  | 1:467:A:GLY:H    | 4                   | 0.38     | 0.16                | 0.44       |
| (3,103) | 1:466:A:PRO:HD3  | 1:467:A:GLY:H    | 4                   | 0.38     | 0.16                | 0.44       |
| (3,775) | 1:531:A:ARG:HA   | 1:534:A:GLN:HG2  | 4                   | 0.37     | 0.2                 | 0.34       |
| (3,775) | 1:531:A:ARG:HA   | 1:534:A:GLN:HG3  | 4                   | 0.37     | 0.2                 | 0.34       |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD11 | 4                   | 0.34     | 0.09                | 0.3        |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD12 | 4                   | 0.34     | 0.09                | 0.3        |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD13 | 4                   | 0.34     | 0.09                | 0.3        |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD21 | 4                   | 0.34     | 0.09                | 0.3        |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD22 | 4                   | 0.34     | 0.09                | 0.3        |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD23 | 4                   | 0.34     | 0.09                | 0.3        |
| (3,882) | 1:548:A:ARG:H    | 1:548:A:ARG:HG2  | 4                   | 0.34     | 0.11                | 0.36       |
| (3,882) | 1:548:A:ARG:H    | 1:548:A:ARG:HG3  | 4                   | 0.34     | 0.11                | 0.36       |
| (3,891) | 1:550:A:LYS:HG2  | 1:551:A:LYS:H    | 4                   | 0.3      | 0.16                | 0.28       |
| (3,891) | 1:550:A:LYS:HG3  | 1:551:A:LYS:H    | 4                   | 0.3      | 0.16                | 0.28       |
| (3,888) | 1:549:A:GLU:HB2  | 1:550:A:LYS:H    | 4                   | 0.29     | 0.15                | 0.26       |
| (3,888) | 1:549:A:GLU:HB3  | 1:550:A:LYS:H    | 4                   | 0.29     | 0.15                | 0.26       |
| (3,879) | 1:547:A:PRO:HB2  | 1:548:A:ARG:H    | 4                   | 0.21     | 0.05                | 0.23       |
| (3,879) | 1:547:A:PRO:HB3  | 1:548:A:ARG:H    | 4                   | 0.21     | 0.05                | 0.23       |
| (3,561) | 1:461:A:SER:HB2  | 1:519:A:TRP:HD1  | 4                   | 0.17     | 0.04                | 0.16       |
| (3,825) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HB   | 4                   | 0.15     | 0.03                | 0.16       |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD11 | 4                   | 0.15     | 0.02                | 0.15       |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD12 | 4                   | 0.15     | 0.02                | 0.15       |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD13 | 4                   | 0.15     | 0.02                | 0.15       |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD21 | 4                   | 0.15     | 0.02                | 0.15       |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD22 | 4                   | 0.15     | 0.02                | 0.15       |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD23 | 4                   | 0.15     | 0.02                | 0.15       |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD11 | 4                   | 0.15     | 0.02                | 0.15       |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD12 | 4                   | 0.15     | 0.02                | 0.15       |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD13 | 4                   | 0.15     | 0.02                | 0.15       |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD21 | 4                   | 0.15     | 0.02                | 0.15       |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD22 | 4                   | 0.15     | 0.02                | 0.15       |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD23 | 4                   | 0.15     | 0.02                | 0.15       |
| (3,52)  | 1:456:A:ILE:HG13 | 1:457:A:VAL:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (3,556) | 1:460:A:ILE:HG21 | 1:519:A:TRP:HA   | 4                   | 0.11     | 0.0                 | 0.11       |
| (3,556) | 1:460:A:ILE:HG22 | 1:519:A:TRP:HA   | 4                   | 0.11     | 0.0                 | 0.11       |
| (3,556) | 1:460:A:ILE:HG23 | 1:519:A:TRP:HA   | 4                   | 0.11     | 0.0                 | 0.11       |
| (3,884) | 1:548:A:ARG:HD2  | 1:549:A:GLU:H    | 3                   | 0.67     | 0.57                | 0.35       |
| (3,884) | 1:548:A:ARG:HD3  | 1:549:A:GLU:H    | 3                   | 0.67     | 0.57                | 0.35       |
| (3,797) | 1:535:A:LYS:HB2  | 1:535:A:LYS:HE2  | 3                   | 0.61     | 0.36                | 0.81       |
| (3,797) | 1:535:A:LYS:HB2  | 1:535:A:LYS:HE3  | 3                   | 0.61     | 0.36                | 0.81       |
| (3,797) | 1:535:A:LYS:HB3  | 1:535:A:LYS:HE2  | 3                   | 0.61     | 0.36                | 0.81       |
| (3,797) | 1:535:A:LYS:HB3  | 1:535:A:LYS:HE3  | 3                   | 0.61     | 0.36                | 0.81       |
| (3,8)   | 1:447:A:THR:HG21 | 1:448:A:GLY:H    | 3                   | 0.56     | 0.14                | 0.49       |
| (3,8)   | 1:447:A:THR:HG22 | 1:448:A:GLY:H    | 3                   | 0.56     | 0.14                | 0.49       |
| (3,8)   | 1:447:A:THR:HG23 | 1:448:A:GLY:H    | 3                   | 0.56     | 0.14                | 0.49       |
| (3,883) | 1:548:A:ARG:HA   | 1:548:A:ARG:HD2  | 3                   | 0.53     | 0.07                | 0.57       |
| (3,883) | 1:548:A:ARG:HA   | 1:548:A:ARG:HD3  | 3                   | 0.53     | 0.07                | 0.57       |
| (3,890) | 1:550:A:LYS:H    | 1:550:A:LYS:HG2  | 3                   | 0.51     | 0.26                | 0.38       |
| (3,890) | 1:550:A:LYS:H    | 1:550:A:LYS:HG3  | 3                   | 0.51     | 0.26                | 0.38       |
| (3,297) | 1:458:A:LYS:HD2  | 1:494:A:HIS:HD2  | 3                   | 0.34     | 0.07                | 0.33       |
| (3,297) | 1:458:A:LYS:HD3  | 1:494:A:HIS:HD2  | 3                   | 0.34     | 0.07                | 0.33       |
| (3,858) | 1:536:A:ILE:HG21 | 1:540:A:ARG:HD2  | 3                   | 0.33     | 0.09                | 0.39       |
| (3,858) | 1:536:A:ILE:HG21 | 1:540:A:ARG:HD3  | 3                   | 0.33     | 0.09                | 0.39       |
| (3,858) | 1:536:A:ILE:HG22 | 1:540:A:ARG:HD2  | 3                   | 0.33     | 0.09                | 0.39       |
| (3,858) | 1:536:A:ILE:HG22 | 1:540:A:ARG:HD3  | 3                   | 0.33     | 0.09                | 0.39       |
| (3,858) | 1:536:A:ILE:HG23 | 1:540:A:ARG:HD2  | 3                   | 0.33     | 0.09                | 0.39       |
| (3,858) | 1:536:A:ILE:HG23 | 1:540:A:ARG:HD3  | 3                   | 0.33     | 0.09                | 0.39       |
| (3,101) | 1:465:A:LEU:HD11 | 1:467:A:GLY:H    | 3                   | 0.31     | 0.18                | 0.21       |
| (3,101) | 1:465:A:LEU:HD12 | 1:467:A:GLY:H    | 3                   | 0.31     | 0.18                | 0.21       |
| (3,101) | 1:465:A:LEU:HD13 | 1:467:A:GLY:H    | 3                   | 0.31     | 0.18                | 0.21       |
| (3,101) | 1:465:A:LEU:HD21 | 1:467:A:GLY:H    | 3                   | 0.31     | 0.18                | 0.21       |
| (3,101) | 1:465:A:LEU:HD22 | 1:467:A:GLY:H    | 3                   | 0.31     | 0.18                | 0.21       |
| (3,101) | 1:465:A:LEU:HD23 | 1:467:A:GLY:H    | 3                   | 0.31     | 0.18                | 0.21       |
| (3,733) | 1:451:A:PHE:HE1  | 1:533:A:TRP:HD1  | 3                   | 0.31     | 0.22                | 0.18       |
| (3,733) | 1:451:A:PHE:HE2  | 1:533:A:TRP:HD1  | 3                   | 0.31     | 0.22                | 0.18       |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD2  | 3                   | 0.31     | 0.11                | 0.31       |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD3  | 3                   | 0.31     | 0.11                | 0.31       |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD2  | 3                   | 0.31     | 0.11                | 0.31       |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD3  | 3                   | 0.31     | 0.11                | 0.31       |
| (3,720) | 1:524:A:LEU:HD11 | 1:532:A:TYR:HD2  | 3                   | 0.24     | 0.08                | 0.28       |
| (3,720) | 1:524:A:LEU:HD12 | 1:532:A:TYR:HD2  | 3                   | 0.24     | 0.08                | 0.28       |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,720) | 1:524:A:LEU:HD13 | 1:532:A:TYR:HD2  | 3                   | 0.24     | 0.08                | 0.28       |
| (3,720) | 1:524:A:LEU:HD21 | 1:532:A:TYR:HD2  | 3                   | 0.24     | 0.08                | 0.28       |
| (3,720) | 1:524:A:LEU:HD22 | 1:532:A:TYR:HD2  | 3                   | 0.24     | 0.08                | 0.28       |
| (3,720) | 1:524:A:LEU:HD23 | 1:532:A:TYR:HD2  | 3                   | 0.24     | 0.08                | 0.28       |
| (1,36)  | 1:500:A:PRO:O    | 1:504:A:GLN:N    | 3                   | 0.23     | 0.1                 | 0.2        |
| (1,38)  | 1:501:A:GLU:O    | 1:505:A:ALA:N    | 3                   | 0.23     | 0.03                | 0.22       |
| (3,689) | 1:526:A:GLY:H    | 1:529:A:GLU:HG2  | 3                   | 0.21     | 0.06                | 0.24       |
| (3,689) | 1:526:A:GLY:H    | 1:529:A:GLU:HG3  | 3                   | 0.21     | 0.06                | 0.24       |
| (3,17)  | 1:450:A:GLN:HA   | 1:451:A:PHE:HD1  | 3                   | 0.2      | 0.08                | 0.15       |
| (3,17)  | 1:450:A:GLN:HA   | 1:451:A:PHE:HD2  | 3                   | 0.2      | 0.08                | 0.15       |
| (3,515) | 1:515:A:LYS:H    | 1:515:A:LYS:HG2  | 3                   | 0.17     | 0.06                | 0.15       |
| (3,515) | 1:515:A:LYS:H    | 1:515:A:LYS:HG3  | 3                   | 0.17     | 0.06                | 0.15       |
| (1,40)  | 1:502:A:ASP:O    | 1:506:A:VAL:N    | 3                   | 0.16     | 0.02                | 0.17       |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD11 | 3                   | 0.16     | 0.02                | 0.16       |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD12 | 3                   | 0.16     | 0.02                | 0.16       |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD13 | 3                   | 0.16     | 0.02                | 0.16       |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD21 | 3                   | 0.16     | 0.02                | 0.16       |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD22 | 3                   | 0.16     | 0.02                | 0.16       |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD23 | 3                   | 0.16     | 0.02                | 0.16       |
| (3,849) | 1:537:A:LEU:HB2  | 1:538:A:VAL:H    | 3                   | 0.16     | 0.05                | 0.13       |
| (3,849) | 1:537:A:LEU:HB3  | 1:538:A:VAL:H    | 3                   | 0.16     | 0.05                | 0.13       |
| (3,369) | 1:481:A:VAL:HG11 | 1:497:A:PHE:HD1  | 3                   | 0.15     | 0.01                | 0.15       |
| (3,369) | 1:481:A:VAL:HG11 | 1:497:A:PHE:HD2  | 3                   | 0.15     | 0.01                | 0.15       |
| (3,369) | 1:481:A:VAL:HG12 | 1:497:A:PHE:HD1  | 3                   | 0.15     | 0.01                | 0.15       |
| (3,369) | 1:481:A:VAL:HG12 | 1:497:A:PHE:HD2  | 3                   | 0.15     | 0.01                | 0.15       |
| (3,369) | 1:481:A:VAL:HG13 | 1:497:A:PHE:HD1  | 3                   | 0.15     | 0.01                | 0.15       |
| (3,369) | 1:481:A:VAL:HG13 | 1:497:A:PHE:HD2  | 3                   | 0.15     | 0.01                | 0.15       |
| (3,113) | 1:469:A:LYS:H    | 1:469:A:LYS:HG2  | 3                   | 0.15     | 0.02                | 0.14       |
| (3,113) | 1:469:A:LYS:H    | 1:469:A:LYS:HG3  | 3                   | 0.15     | 0.02                | 0.14       |
| (3,34)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:HA2  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,34)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:HA3  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,34)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:HA2  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,34)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:HA3  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,34)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:HA2  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,34)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:HA3  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,34)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:HA2  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,34)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:HA3  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,34)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:HA2  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,34)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:HA3  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,34)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:HA2  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,34)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:HA3  | 3                   | 0.13     | 0.03                | 0.13       |
| (3,179) | 1:478:A:ILE:HA   | 1:478:A:ILE:HG12 | 3                   | 0.11     | 0.0                 | 0.11       |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,179) | 1:478:A:ILE:HA   | 1:478:A:ILE:HG13 | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,237) | 1:488:A:GLU:H    | 1:488:A:GLU:HB2  | 3                   | 0.11     | 0.01                | 0.1        |
| (3,237) | 1:488:A:GLU:H    | 1:488:A:GLU:HB3  | 3                   | 0.11     | 0.01                | 0.1        |
| (3,598) | 1:519:A:TRP:HE1  | 1:520:A:LYS:HB2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (3,598) | 1:519:A:TRP:HE1  | 1:520:A:LYS:HB3  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,73)  | 1:532:A:TYR:O    | 1:536:A:ILE:H    | 3                   | 0.1      | 0.0                 | 0.1        |
| (3,489) | 1:510:A:TYR:HB3  | 1:512:A:GLU:H    | 3                   | 0.1      | 0.0                 | 0.1        |
| (3,752) | 1:496:A:ARG:HG2  | 1:533:A:TRP:HZ2  | 2                   | 1.63     | 0.03                | 1.63       |
| (3,752) | 1:496:A:ARG:HG3  | 1:533:A:TRP:HZ2  | 2                   | 1.63     | 0.03                | 1.63       |
| (3,791) | 1:535:A:LYS:H    | 1:535:A:LYS:HG2  | 2                   | 1.04     | 0.0                 | 1.04       |
| (3,791) | 1:535:A:LYS:H    | 1:535:A:LYS:HG3  | 2                   | 1.04     | 0.0                 | 1.04       |
| (3,13)  | 1:450:A:GLN:H    | 1:450:A:GLN:HG2  | 2                   | 0.97     | 0.26                | 0.97       |
| (3,13)  | 1:450:A:GLN:H    | 1:450:A:GLN:HG3  | 2                   | 0.97     | 0.26                | 0.97       |
| (3,751) | 1:496:A:ARG:HG2  | 1:533:A:TRP:HH2  | 2                   | 0.97     | 0.39                | 0.97       |
| (3,751) | 1:496:A:ARG:HG3  | 1:533:A:TRP:HH2  | 2                   | 0.97     | 0.39                | 0.97       |
| (3,513) | 1:515:A:LYS:H    | 1:515:A:LYS:HD2  | 2                   | 0.62     | 0.26                | 0.62       |
| (3,513) | 1:515:A:LYS:H    | 1:515:A:LYS:HD3  | 2                   | 0.62     | 0.26                | 0.62       |
| (3,859) | 1:539:A:ASP:HB3  | 1:540:A:ARG:HD2  | 2                   | 0.54     | 0.04                | 0.54       |
| (3,859) | 1:539:A:ASP:HB3  | 1:540:A:ARG:HD3  | 2                   | 0.54     | 0.04                | 0.54       |
| (3,904) | 1:555:A:GLU:HB2  | 1:556:A:LYS:H    | 2                   | 0.52     | 0.01                | 0.52       |
| (3,904) | 1:555:A:GLU:HB3  | 1:556:A:LYS:H    | 2                   | 0.52     | 0.01                | 0.52       |
| (3,793) | 1:535:A:LYS:H    | 1:535:A:LYS:HG2  | 2                   | 0.44     | 0.0                 | 0.44       |
| (3,793) | 1:535:A:LYS:H    | 1:535:A:LYS:HG3  | 2                   | 0.44     | 0.0                 | 0.44       |
| (3,16)  | 1:450:A:GLN:H    | 1:451:A:PHE:HD1  | 2                   | 0.37     | 0.21                | 0.37       |
| (3,16)  | 1:450:A:GLN:H    | 1:451:A:PHE:HD2  | 2                   | 0.37     | 0.21                | 0.37       |
| (3,786) | 1:532:A:TYR:HE1  | 1:535:A:LYS:HD2  | 2                   | 0.36     | 0.01                | 0.36       |
| (3,786) | 1:532:A:TYR:HE1  | 1:535:A:LYS:HD3  | 2                   | 0.36     | 0.01                | 0.36       |
| (3,496) | 1:513:A:ILE:H    | 1:513:A:ILE:HD11 | 2                   | 0.33     | 0.04                | 0.33       |
| (3,496) | 1:513:A:ILE:H    | 1:513:A:ILE:HD12 | 2                   | 0.33     | 0.04                | 0.33       |
| (3,496) | 1:513:A:ILE:H    | 1:513:A:ILE:HD13 | 2                   | 0.33     | 0.04                | 0.33       |
| (3,695) | 1:451:A:PHE:HE1  | 1:530:A:GLN:HA   | 2                   | 0.26     | 0.02                | 0.26       |
| (3,695) | 1:451:A:PHE:HE2  | 1:530:A:GLN:HA   | 2                   | 0.26     | 0.02                | 0.26       |
| (3,183) | 1:478:A:ILE:HB   | 1:479:A:SER:HB2  | 2                   | 0.24     | 0.08                | 0.24       |
| (3,183) | 1:478:A:ILE:HB   | 1:479:A:SER:HB3  | 2                   | 0.24     | 0.08                | 0.24       |
| (1,45)  | 1:505:A:ALA:O    | 1:509:A:ALA:H    | 2                   | 0.2      | 0.07                | 0.2        |
| (3,361) | 1:457:A:VAL:HG11 | 1:497:A:PHE:HE1  | 2                   | 0.18     | 0.01                | 0.18       |
| (3,361) | 1:457:A:VAL:HG11 | 1:497:A:PHE:HE2  | 2                   | 0.18     | 0.01                | 0.18       |
| (3,361) | 1:457:A:VAL:HG12 | 1:497:A:PHE:HE1  | 2                   | 0.18     | 0.01                | 0.18       |
| (3,361) | 1:457:A:VAL:HG12 | 1:497:A:PHE:HE2  | 2                   | 0.18     | 0.01                | 0.18       |
| (3,361) | 1:457:A:VAL:HG13 | 1:497:A:PHE:HE1  | 2                   | 0.18     | 0.01                | 0.18       |
| (3,361) | 1:457:A:VAL:HG13 | 1:497:A:PHE:HE2  | 2                   | 0.18     | 0.01                | 0.18       |
| (3,361) | 1:457:A:VAL:HG21 | 1:497:A:PHE:HE1  | 2                   | 0.18     | 0.01                | 0.18       |

*Continued on next page...*

Continued from previous page...

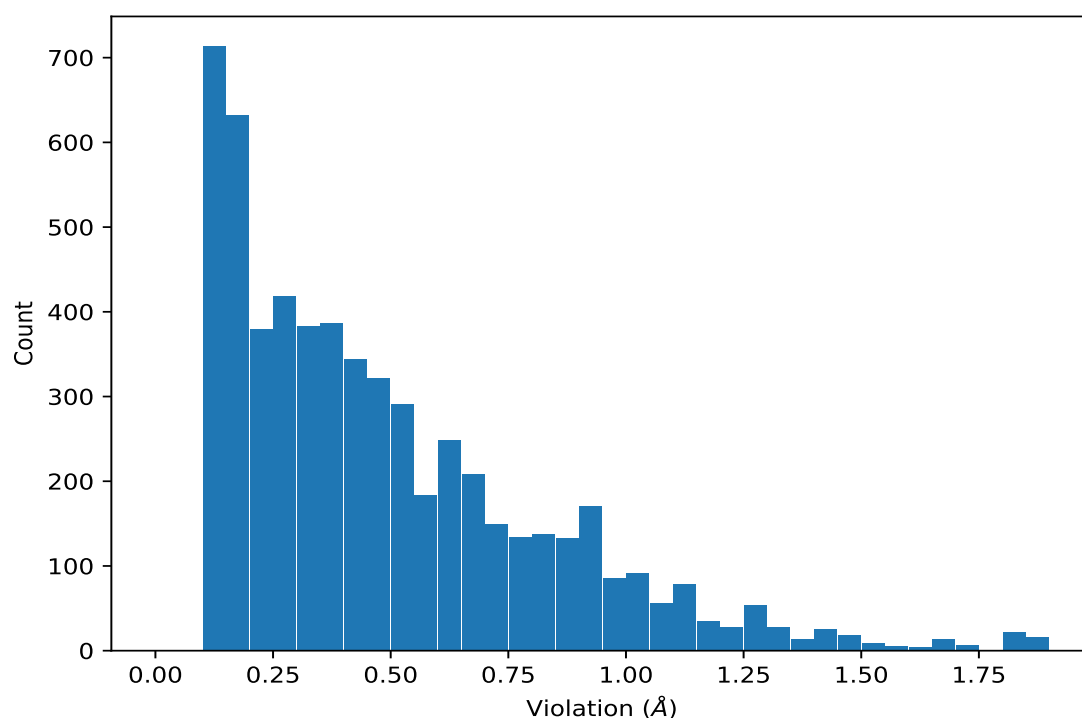
| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (3,361) | 1:457:A:VAL:HG21 | 1:497:A:PHE:HE2  | 2                   | 0.18     | 0.01                | 0.18       |
| (3,361) | 1:457:A:VAL:HG22 | 1:497:A:PHE:HE1  | 2                   | 0.18     | 0.01                | 0.18       |
| (3,361) | 1:457:A:VAL:HG22 | 1:497:A:PHE:HE2  | 2                   | 0.18     | 0.01                | 0.18       |
| (3,361) | 1:457:A:VAL:HG23 | 1:497:A:PHE:HE1  | 2                   | 0.18     | 0.01                | 0.18       |
| (3,361) | 1:457:A:VAL:HG23 | 1:497:A:PHE:HE2  | 2                   | 0.18     | 0.01                | 0.18       |
| (3,730) | 1:451:A:PHE:HZ   | 1:533:A:TRP:HD1  | 2                   | 0.18     | 0.08                | 0.18       |
| (3,333) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HA   | 2                   | 0.17     | 0.06                | 0.17       |
| (3,333) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HA   | 2                   | 0.17     | 0.06                | 0.17       |
| (3,333) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HA   | 2                   | 0.17     | 0.06                | 0.17       |
| (3,447) | 1:504:A:GLN:HG2  | 1:508:A:ASN:HD21 | 2                   | 0.17     | 0.05                | 0.17       |
| (3,447) | 1:504:A:GLN:HG3  | 1:508:A:ASN:HD21 | 2                   | 0.17     | 0.05                | 0.17       |
| (3,447) | 1:504:A:GLN:HG2  | 1:508:A:ASN:HD22 | 2                   | 0.17     | 0.05                | 0.17       |
| (3,447) | 1:504:A:GLN:HG3  | 1:508:A:ASN:HD22 | 2                   | 0.17     | 0.05                | 0.17       |
| (3,261) | 1:491:A:THR:H    | 1:492:A:GLU:HG2  | 2                   | 0.16     | 0.04                | 0.16       |
| (3,261) | 1:491:A:THR:H    | 1:492:A:GLU:HG3  | 2                   | 0.16     | 0.04                | 0.16       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD11 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD12 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD13 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD21 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD22 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD23 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD11 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD12 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD13 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD21 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD22 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD23 | 2                   | 0.15     | 0.04                | 0.15       |
| (3,280) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HA   | 2                   | 0.15     | 0.0                 | 0.15       |
| (3,280) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HA   | 2                   | 0.15     | 0.0                 | 0.15       |

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

### 9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



### 9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2 | 4        | 1.89          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3 | 4        | 1.89          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2 | 4        | 1.89          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3 | 4        | 1.89          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2 | 7        | 1.87          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2 | 7        | 1.87          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2 | 7        | 1.87          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3 | 7        | 1.87          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3 | 7        | 1.87          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3 | 7        | 1.87          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2 | 12       | 1.86          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2 | 12       | 1.86          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2 | 12       | 1.86          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3 | 12       | 1.86          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3 | 12       | 1.86          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3 | 12       | 1.86          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (3,893) | 1:552:A:ARG:H    | 1:552:A:ARG:HD2 | 18       | 1.84          |
| (3,893) | 1:552:A:ARG:H    | 1:552:A:ARG:HD3 | 18       | 1.84          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA  | 17       | 1.84          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2 | 20       | 1.84          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3 | 20       | 1.84          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2 | 20       | 1.84          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3 | 20       | 1.84          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA  | 6        | 1.83          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2 | 5        | 1.83          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2 | 5        | 1.83          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2 | 5        | 1.83          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3 | 5        | 1.83          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3 | 5        | 1.83          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3 | 5        | 1.83          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2 | 14       | 1.82          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2 | 14       | 1.82          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2 | 14       | 1.82          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3 | 14       | 1.82          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3 | 14       | 1.82          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3 | 14       | 1.82          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA  | 14       | 1.8           |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA  | 20       | 1.8           |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA  | 3        | 1.74          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA  | 9        | 1.74          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA  | 1        | 1.73          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA  | 12       | 1.71          |
| (3,900) | 1:554:A:THR:HG21 | 1:555:A:GLU:H   | 10       | 1.7           |
| (3,900) | 1:554:A:THR:HG22 | 1:555:A:GLU:H   | 10       | 1.7           |
| (3,900) | 1:554:A:THR:HG23 | 1:555:A:GLU:H   | 10       | 1.7           |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA  | 5        | 1.69          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA  | 11       | 1.69          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2 | 18       | 1.67          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2 | 18       | 1.67          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2 | 18       | 1.67          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3 | 18       | 1.67          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3 | 18       | 1.67          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3 | 18       | 1.67          |
| (3,752) | 1:496:A:ARG:HG2  | 1:533:A:TRP:HZ2 | 20       | 1.66          |
| (3,752) | 1:496:A:ARG:HG3  | 1:533:A:TRP:HZ2 | 20       | 1.66          |
| (3,900) | 1:554:A:THR:HG21 | 1:555:A:GLU:H   | 11       | 1.65          |
| (3,900) | 1:554:A:THR:HG22 | 1:555:A:GLU:H   | 11       | 1.65          |
| (3,900) | 1:554:A:THR:HG23 | 1:555:A:GLU:H   | 11       | 1.65          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA   | 16       | 1.65          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA   | 8        | 1.64          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA   | 13       | 1.61          |
| (3,752) | 1:496:A:ARG:HG2  | 1:533:A:TRP:HZ2  | 15       | 1.6           |
| (3,752) | 1:496:A:ARG:HG3  | 1:533:A:TRP:HZ2  | 15       | 1.6           |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA   | 19       | 1.59          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD21 | 5        | 1.58          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD22 | 5        | 1.58          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2  | 10       | 1.56          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 10       | 1.56          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 7        | 1.54          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 7        | 1.54          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 7        | 1.54          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA   | 18       | 1.54          |
| (3,874) | 1:545:A:ASN:H    | 1:546:A:GLN:H    | 15       | 1.51          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 18       | 1.51          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 18       | 1.51          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 18       | 1.51          |
| (3,1)   | 1:445:A:ASN:HB2  | 1:446:A:ALA:H    | 9        | 1.5           |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 5        | 1.49          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 5        | 1.49          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 5        | 1.49          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 19       | 1.48          |
| (3,884) | 1:548:A:ARG:HD2  | 1:549:A:GLU:H    | 15       | 1.47          |
| (3,884) | 1:548:A:ARG:HD3  | 1:549:A:GLU:H    | 15       | 1.47          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA   | 15       | 1.47          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 13       | 1.47          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 13       | 1.47          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 13       | 1.47          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 13       | 1.47          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 13       | 1.47          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 13       | 1.47          |
| (3,893) | 1:552:A:ARG:H    | 1:552:A:ARG:HD2  | 12       | 1.46          |
| (3,893) | 1:552:A:ARG:H    | 1:552:A:ARG:HD3  | 12       | 1.46          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 4        | 1.45          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 4        | 1.45          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 4        | 1.45          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 16       | 1.44          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG21 | 10       | 1.43          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG22 | 10       | 1.43          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG23 | 10       | 1.43          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 14       | 1.43          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,1)   | 1:445:A:ASN:HB2  | 1:446:A:ALA:H    | 5        | 1.43          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 8        | 1.42          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 8        | 1.42          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 8        | 1.42          |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD2  | 19       | 1.41          |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD3  | 19       | 1.41          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 12       | 1.41          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 12       | 1.41          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 12       | 1.41          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 4        | 1.41          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 4        | 1.41          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 3        | 1.4           |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 3        | 1.4           |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 3        | 1.4           |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 6        | 1.4           |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 6        | 1.4           |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 6        | 1.4           |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 19       | 1.4           |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 19       | 1.4           |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 19       | 1.4           |
| (3,899) | 1:554:A:THR:H    | 1:555:A:GLU:H    | 15       | 1.39          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA   | 4        | 1.39          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 16       | 1.38          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 16       | 1.38          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 16       | 1.38          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 16       | 1.38          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 16       | 1.38          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 16       | 1.38          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2  | 4        | 1.36          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 4        | 1.36          |
| (3,751) | 1:496:A:ARG:HG2  | 1:533:A:TRP:HH2  | 20       | 1.35          |
| (3,751) | 1:496:A:ARG:HG3  | 1:533:A:TRP:HH2  | 20       | 1.35          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 11       | 1.35          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 11       | 1.35          |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 17       | 1.34          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 9        | 1.33          |
| (3,913) | 1:558:A:ILE:HG21 | 1:559:A:THR:H    | 15       | 1.32          |
| (3,913) | 1:558:A:ILE:HG22 | 1:559:A:THR:H    | 15       | 1.32          |
| (3,913) | 1:558:A:ILE:HG23 | 1:559:A:THR:H    | 15       | 1.32          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 16       | 1.32          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2  | 17       | 1.31          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 17       | 1.31          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 10       | 1.31          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 10       | 1.31          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 10       | 1.31          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 13       | 1.31          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 13       | 1.31          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 13       | 1.31          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 6        | 1.31          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 11       | 1.31          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 5        | 1.3           |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 5        | 1.3           |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 9        | 1.3           |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 9        | 1.3           |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 9        | 1.3           |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 14       | 1.3           |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 14       | 1.3           |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 14       | 1.3           |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 17       | 1.3           |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 17       | 1.3           |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 17       | 1.3           |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 12       | 1.3           |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 2        | 1.29          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 2        | 1.29          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 4        | 1.29          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 4        | 1.29          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 9        | 1.29          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 9        | 1.29          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 10       | 1.29          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 10       | 1.29          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 17       | 1.29          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 17       | 1.29          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 11       | 1.29          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 11       | 1.29          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 11       | 1.29          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 7        | 1.29          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 8        | 1.29          |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 5        | 1.29          |
| (3,896) | 1:553:A:GLY:H    | 1:554:A:THR:H    | 10       | 1.28          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 3        | 1.28          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 3        | 1.28          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 11       | 1.28          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 11       | 1.28          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 12       | 1.28          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 12       | 1.28          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 5        | 1.28          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 5        | 1.28          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 5        | 1.28          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 5        | 1.28          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 5        | 1.28          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 5        | 1.28          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 1        | 1.27          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 1        | 1.27          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 13       | 1.27          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 13       | 1.27          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 15       | 1.27          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 15       | 1.27          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 15       | 1.27          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA   | 2        | 1.27          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 7        | 1.26          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 7        | 1.26          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 15       | 1.26          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 15       | 1.26          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA   | 7        | 1.26          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 1        | 1.26          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 6        | 1.26          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 6        | 1.26          |
| (3,889) | 1:549:A:GLU:HG2  | 1:550:A:LYS:H    | 15       | 1.25          |
| (3,889) | 1:549:A:GLU:HG3  | 1:550:A:LYS:H    | 15       | 1.25          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 8        | 1.25          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 8        | 1.25          |
| (3,543) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HA   | 10       | 1.25          |
| (3,436) | 1:479:A:SER:HB2  | 1:506:A:VAL:HB   | 7        | 1.25          |
| (3,436) | 1:479:A:SER:HB3  | 1:506:A:VAL:HB   | 7        | 1.25          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 8        | 1.25          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 8        | 1.25          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 6        | 1.24          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 6        | 1.24          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 18       | 1.24          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 18       | 1.24          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 20       | 1.24          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 20       | 1.24          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 1        | 1.24          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 1        | 1.24          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 1        | 1.24          |
| (3,1)   | 1:445:A:ASN:HB2  | 1:446:A:ALA:H    | 17       | 1.24          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 3        | 1.23          |
| (3,13)  | 1:450:A:GLN:H    | 1:450:A:GLN:HG2  | 20       | 1.23          |
| (3,13)  | 1:450:A:GLN:H    | 1:450:A:GLN:HG3  | 20       | 1.23          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 14       | 1.22          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 14       | 1.22          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 19       | 1.22          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 19       | 1.22          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 6        | 1.22          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 6        | 1.22          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 6        | 1.22          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 6        | 1.22          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 6        | 1.22          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 6        | 1.22          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 20       | 1.21          |
| (3,642) | 1:523:A:ILE:HA   | 1:523:A:ILE:HD11 | 13       | 1.2           |
| (3,642) | 1:523:A:ILE:HA   | 1:523:A:ILE:HD12 | 13       | 1.2           |
| (3,642) | 1:523:A:ILE:HA   | 1:523:A:ILE:HD13 | 13       | 1.2           |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 19       | 1.2           |
| (3,900) | 1:554:A:THR:HG21 | 1:555:A:GLU:H    | 6        | 1.19          |
| (3,900) | 1:554:A:THR:HG22 | 1:555:A:GLU:H    | 6        | 1.19          |
| (3,900) | 1:554:A:THR:HG23 | 1:555:A:GLU:H    | 6        | 1.19          |
| (3,681) | 1:524:A:LEU:HB2  | 1:529:A:GLU:HA   | 16       | 1.19          |
| (3,681) | 1:524:A:LEU:HB3  | 1:529:A:GLU:HA   | 16       | 1.19          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 7        | 1.19          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 2        | 1.19          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 2        | 1.19          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 2        | 1.19          |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 16       | 1.19          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG21 | 17       | 1.18          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG22 | 17       | 1.18          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG23 | 17       | 1.18          |
| (3,619) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HG   | 8        | 1.16          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 3        | 1.16          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 3        | 1.16          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD21 | 14       | 1.15          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD22 | 14       | 1.15          |
| (3,863) | 1:541:A:GLN:HA   | 1:541:A:GLN:HE21 | 20       | 1.15          |
| (3,863) | 1:541:A:GLN:HA   | 1:541:A:GLN:HE22 | 20       | 1.15          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 5        | 1.15          |
| (3,1)   | 1:445:A:ASN:HB2  | 1:446:A:ALA:H    | 3        | 1.15          |
| (3,1)   | 1:445:A:ASN:HB2  | 1:446:A:ALA:H    | 14       | 1.15          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG2  | 1        | 1.14          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG3  | 1        | 1.14          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 11       | 1.14          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 16       | 1.14          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 16       | 1.14          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 16       | 1.14          |
| (3,550) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HE1  | 20       | 1.14          |
| (3,550) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HE1  | 20       | 1.14          |
| (3,550) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HE1  | 20       | 1.14          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 18       | 1.14          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 17       | 1.14          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 17       | 1.14          |
| (3,911) | 1:558:A:ILE:HB   | 1:559:A:THR:H    | 7        | 1.13          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 10       | 1.13          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 3        | 1.12          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 3        | 1.12          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 18       | 1.12          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 18       | 1.12          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 16       | 1.12          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 16       | 1.12          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 19       | 1.12          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 19       | 1.12          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 19       | 1.12          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 19       | 1.12          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 19       | 1.12          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 19       | 1.12          |
| (3,1)   | 1:445:A:ASN:HB2  | 1:446:A:ALA:H    | 16       | 1.12          |
| (3,900) | 1:554:A:THR:HG21 | 1:555:A:GLU:H    | 8        | 1.11          |
| (3,900) | 1:554:A:THR:HG22 | 1:555:A:GLU:H    | 8        | 1.11          |
| (3,900) | 1:554:A:THR:HG23 | 1:555:A:GLU:H    | 8        | 1.11          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2  | 7        | 1.11          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 7        | 1.11          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD21 | 9        | 1.11          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD22 | 9        | 1.11          |
| (3,617) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HG   | 8        | 1.11          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 7        | 1.11          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 7        | 1.11          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 7        | 1.11          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 7        | 1.11          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 7        | 1.11          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 7        | 1.11          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 7        | 1.11          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 7        | 1.11          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 7        | 1.11          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 7        | 1.11          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 7        | 1.11          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 7        | 1.11          |
| (3,913) | 1:558:A:ILE:HG21 | 1:559:A:THR:H    | 5        | 1.1           |
| (3,913) | 1:558:A:ILE:HG22 | 1:559:A:THR:H    | 5        | 1.1           |
| (3,913) | 1:558:A:ILE:HG23 | 1:559:A:THR:H    | 5        | 1.1           |
| (3,889) | 1:549:A:GLU:HG2  | 1:550:A:LYS:H    | 4        | 1.1           |
| (3,889) | 1:549:A:GLU:HG3  | 1:550:A:LYS:H    | 4        | 1.1           |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 20       | 1.1           |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 20       | 1.1           |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 20       | 1.1           |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 20       | 1.1           |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 20       | 1.1           |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 20       | 1.1           |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 20       | 1.1           |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 6        | 1.1           |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 6        | 1.1           |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 15       | 1.1           |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 15       | 1.1           |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 15       | 1.1           |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 15       | 1.1           |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 15       | 1.1           |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 15       | 1.1           |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 15       | 1.1           |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 15       | 1.1           |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 15       | 1.1           |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 15       | 1.1           |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 15       | 1.1           |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 15       | 1.1           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 15       | 1.1           |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 12       | 1.1           |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 12       | 1.1           |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 12       | 1.1           |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 12       | 1.1           |
| (3,900) | 1:554:A:THR:HG21 | 1:555:A:GLU:H    | 17       | 1.09          |
| (3,900) | 1:554:A:THR:HG22 | 1:555:A:GLU:H    | 17       | 1.09          |
| (3,900) | 1:554:A:THR:HG23 | 1:555:A:GLU:H    | 17       | 1.09          |
| (3,436) | 1:479:A:SER:HB2  | 1:506:A:VAL:HB   | 15       | 1.09          |
| (3,436) | 1:479:A:SER:HB3  | 1:506:A:VAL:HB   | 15       | 1.09          |
| (3,874) | 1:545:A:ASN:H    | 1:546:A:GLN:H    | 12       | 1.08          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 2        | 1.08          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 18       | 1.07          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 18       | 1.07          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 6        | 1.07          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 12       | 1.07          |
| (3,913) | 1:558:A:ILE:HG21 | 1:559:A:THR:H    | 4        | 1.06          |
| (3,913) | 1:558:A:ILE:HG22 | 1:559:A:THR:H    | 4        | 1.06          |
| (3,913) | 1:558:A:ILE:HG23 | 1:559:A:THR:H    | 4        | 1.06          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 8        | 1.06          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 8        | 1.06          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 5        | 1.06          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 5        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 8        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 8        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 8        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 8        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 8        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 8        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 8        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 8        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 8        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 8        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 8        | 1.06          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 8        | 1.06          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 20       | 1.06          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 20       | 1.06          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 20       | 1.06          |
| (3,899) | 1:554:A:THR:H    | 1:555:A:GLU:H    | 18       | 1.05          |
| (3,619) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HG   | 3        | 1.05          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 13       | 1.05          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 14       | 1.05          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 18       | 1.05          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 8        | 1.05          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 8        | 1.05          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 11       | 1.05          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 11       | 1.05          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 11       | 1.05          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 11       | 1.05          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 11       | 1.05          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 11       | 1.05          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 11       | 1.05          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 11       | 1.05          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 11       | 1.05          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 11       | 1.05          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 11       | 1.05          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 11       | 1.05          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 14       | 1.05          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 14       | 1.05          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 14       | 1.05          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 14       | 1.05          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG21 | 16       | 1.04          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG22 | 16       | 1.04          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG23 | 16       | 1.04          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG2  | 5        | 1.04          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG3  | 5        | 1.04          |
| (3,791) | 1:535:A:LYS:H    | 1:535:A:LYS:HG2  | 14       | 1.04          |
| (3,791) | 1:535:A:LYS:H    | 1:535:A:LYS:HG3  | 14       | 1.04          |
| (3,791) | 1:535:A:LYS:H    | 1:535:A:LYS:HG2  | 19       | 1.04          |
| (3,791) | 1:535:A:LYS:H    | 1:535:A:LYS:HG3  | 19       | 1.04          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 1        | 1.04          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 1        | 1.04          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 1        | 1.04          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 1        | 1.04          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 1        | 1.04          |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 11       | 1.04          |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG2  | 12       | 1.03          |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG3  | 12       | 1.03          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 18       | 1.03          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 18       | 1.03          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 18       | 1.03          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 18       | 1.03          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 18       | 1.03          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 18       | 1.03          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 18       | 1.03          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 18       | 1.03          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 18       | 1.03          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 18       | 1.03          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 18       | 1.03          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 18       | 1.03          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 20       | 1.03          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 5        | 1.03          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 2        | 1.02          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 10       | 1.02          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 10       | 1.02          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 10       | 1.02          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 10       | 1.02          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 10       | 1.02          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 10       | 1.02          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 13       | 1.02          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 17       | 1.02          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 11       | 1.02          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 11       | 1.02          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 11       | 1.02          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 11       | 1.02          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 11       | 1.02          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 11       | 1.02          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 9        | 1.01          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 9        | 1.01          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 9        | 1.01          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 9        | 1.01          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 9        | 1.01          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 9        | 1.01          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 9        | 1.01          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 9        | 1.01          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 9        | 1.01          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 9        | 1.01          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 9        | 1.01          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 9        | 1.01          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 14       | 1.01          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 14       | 1.01          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 19       | 1.01          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 19       | 1.01          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 19       | 1.01          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 19       | 1.01          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 19       | 1.01          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 19       | 1.01          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 19       | 1.01          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 19       | 1.01          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 19       | 1.01          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 19       | 1.01          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 19       | 1.01          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 19       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 13       | 1.01          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG2  | 20       | 1.0           |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG3  | 20       | 1.0           |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 13       | 1.0           |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 13       | 1.0           |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 13       | 1.0           |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 13       | 1.0           |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 4        | 1.0           |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 4        | 1.0           |
| (3,899) | 1:554:A:THR:H    | 1:555:A:GLU:H    | 11       | 0.99          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 3        | 0.99          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 19       | 0.99          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 2        | 0.99          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 2        | 0.99          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 14       | 0.99          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 14       | 0.99          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 14       | 0.99          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 14       | 0.99          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 2        | 0.99          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 16       | 0.99          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 14       | 0.98          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 14       | 0.98          |
| (3,619) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HG   | 5        | 0.98          |
| (3,505) | 1:514:A:ASN:HA   | 1:514:A:ASN:HD21 | 17       | 0.98          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2 | 3        | 0.98          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2 | 7        | 0.98          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2 | 14       | 0.98          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2 | 20       | 0.98          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H   | 4        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H   | 8        | 0.98          |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG2 | 3        | 0.97          |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG3 | 3        | 0.97          |
| (3,899) | 1:554:A:THR:H    | 1:555:A:GLU:H   | 10       | 0.97          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2 | 14       | 0.97          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3 | 14       | 0.97          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ  | 5        | 0.97          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ  | 5        | 0.97          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2 | 1        | 0.97          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2 | 1        | 0.97          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2 | 1        | 0.97          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3 | 1        | 0.97          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3 | 1        | 0.97          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3 | 1        | 0.97          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB  | 8        | 0.96          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 3        | 0.96          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 9        | 0.96          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 15       | 0.96          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 4        | 0.96          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 4        | 0.96          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 9        | 0.96          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 9        | 0.96          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 9        | 0.96          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 9        | 0.96          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 9        | 0.96          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 9        | 0.96          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 1        | 0.95          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 17       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 15       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 15       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 15       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 15       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 15       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 15       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 15       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 15       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 15       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 15       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 15       | 0.95          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 15       | 0.95          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 12       | 0.95          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 16       | 0.95          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 16       | 0.95          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 19       | 0.95          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 15       | 0.94          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 6        | 0.94          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 11       | 0.94          |
| (3,436) | 1:479:A:SER:HB2  | 1:506:A:VAL:HB   | 19       | 0.94          |
| (3,436) | 1:479:A:SER:HB3  | 1:506:A:VAL:HB   | 19       | 0.94          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 12       | 0.94          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 12       | 0.94          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 4        | 0.94          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 4        | 0.94          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 4        | 0.94          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 4        | 0.94          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 4        | 0.94          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 4        | 0.94          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 4        | 0.94          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 4        | 0.94          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 4        | 0.94          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 4        | 0.94          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 4        | 0.94          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 4        | 0.94          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 10       | 0.94          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 10       | 0.94          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 10       | 0.94          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 10       | 0.94          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 10       | 0.94          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 10       | 0.94          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 19       | 0.93          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 19       | 0.93          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 12       | 0.93          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 15       | 0.93          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 15       | 0.93          |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD2  | 3        | 0.92          |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD3  | 3        | 0.92          |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD2  | 6        | 0.92          |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD3  | 6        | 0.92          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 9        | 0.92          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 18       | 0.92          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 18       | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 8        | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 8        | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 8        | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 8        | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 8        | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 8        | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 8        | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 8        | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 8        | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 8        | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 8        | 0.92          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 8        | 0.92          |
| (3,617) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HG   | 3        | 0.92          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 9        | 0.92          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 9        | 0.92          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 1        | 0.92          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 1        | 0.92          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 1        | 0.92          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1 | 9        | 0.92          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2 | 9        | 0.92          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ  | 7        | 0.92          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ  | 7        | 0.92          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2 | 10       | 0.92          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2 | 10       | 0.92          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2 | 10       | 0.92          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3 | 10       | 0.92          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3 | 10       | 0.92          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3 | 10       | 0.92          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2 | 6        | 0.92          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2 | 6        | 0.92          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2 | 6        | 0.92          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3 | 6        | 0.92          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3 | 6        | 0.92          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3 | 6        | 0.92          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2 | 6        | 0.92          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2 | 6        | 0.92          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2 | 6        | 0.92          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3 | 6        | 0.92          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3 | 6        | 0.92          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3 | 6        | 0.92          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H   | 15       | 0.92          |
| (3,874) | 1:545:A:ASN:H    | 1:546:A:GLN:H   | 2        | 0.91          |
| (3,797) | 1:535:A:LYS:HB2  | 1:535:A:LYS:HE2 | 14       | 0.91          |
| (3,797) | 1:535:A:LYS:HB2  | 1:535:A:LYS:HE3 | 14       | 0.91          |
| (3,797) | 1:535:A:LYS:HB3  | 1:535:A:LYS:HE2 | 14       | 0.91          |
| (3,797) | 1:535:A:LYS:HB3  | 1:535:A:LYS:HE3 | 14       | 0.91          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3 | 9        | 0.91          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1 | 7        | 0.91          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2 | 7        | 0.91          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 18       | 0.91          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 18       | 0.91          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 9        | 0.91          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 9        | 0.91          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 10       | 0.91          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 10       | 0.91          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 8        | 0.91          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 8        | 0.91          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 8        | 0.91          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 8        | 0.91          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 8        | 0.91          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 8        | 0.91          |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 19       | 0.91          |
| (3,731) | 1:451:A:PHE:HD1  | 1:533:A:TRP:HB3  | 12       | 0.9           |
| (3,731) | 1:451:A:PHE:HD2  | 1:533:A:TRP:HB3  | 12       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 18       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 18       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 18       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 18       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 18       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 18       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 18       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 18       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 18       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 18       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 18       | 0.9           |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 18       | 0.9           |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 5        | 0.9           |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 5        | 0.9           |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 5        | 0.9           |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 5        | 0.9           |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 5        | 0.9           |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 5        | 0.9           |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 16       | 0.9           |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 16       | 0.9           |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 16       | 0.9           |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 16       | 0.9           |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 16       | 0.9           |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 16       | 0.9           |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 18       | 0.9           |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 18       | 0.9           |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 18       | 0.9           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 18       | 0.9           |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 18       | 0.9           |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 18       | 0.9           |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 2        | 0.9           |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 2        | 0.9           |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 13       | 0.9           |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 13       | 0.9           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 6        | 0.9           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 15       | 0.9           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 15       | 0.9           |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 15       | 0.9           |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 15       | 0.9           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 15       | 0.9           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 15       | 0.9           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 15       | 0.9           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 15       | 0.9           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 15       | 0.9           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 15       | 0.9           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 15       | 0.9           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 15       | 0.9           |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG21 | 19       | 0.89          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG22 | 19       | 0.89          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG23 | 19       | 0.89          |
| (3,889) | 1:549:A:GLU:HG2  | 1:550:A:LYS:H    | 17       | 0.89          |
| (3,889) | 1:549:A:GLU:HG3  | 1:550:A:LYS:H    | 17       | 0.89          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 15       | 0.89          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 15       | 0.89          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 15       | 0.89          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 15       | 0.89          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 15       | 0.89          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 15       | 0.89          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 15       | 0.89          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 15       | 0.89          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 15       | 0.89          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 15       | 0.89          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 15       | 0.89          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 15       | 0.89          |
| (3,617) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HG   | 5        | 0.89          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 18       | 0.89          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 18       | 0.89          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG21 | 2        | 0.88          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG22 | 2        | 0.88          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG23 | 2        | 0.88          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 14       | 0.88          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 3        | 0.88          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 3        | 0.88          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 1        | 0.88          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 1        | 0.88          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 1        | 0.88          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 1        | 0.88          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 1        | 0.88          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 1        | 0.88          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 16       | 0.88          |
| (3,513) | 1:515:A:LYS:H    | 1:515:A:LYS:HD2  | 17       | 0.88          |
| (3,513) | 1:515:A:LYS:H    | 1:515:A:LYS:HD3  | 17       | 0.88          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE21 | 9        | 0.88          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE22 | 9        | 0.88          |
| (3,890) | 1:550:A:LYS:H    | 1:550:A:LYS:HG2  | 7        | 0.87          |
| (3,890) | 1:550:A:LYS:H    | 1:550:A:LYS:HG3  | 7        | 0.87          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD21 | 1        | 0.87          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD22 | 1        | 0.87          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 15       | 0.87          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 20       | 0.87          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 20       | 0.87          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 20       | 0.87          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 20       | 0.87          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 20       | 0.87          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 20       | 0.87          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 20       | 0.87          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 20       | 0.87          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 20       | 0.87          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 20       | 0.87          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 20       | 0.87          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 20       | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 4        | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 4        | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 4        | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 4        | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 4        | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 4        | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 4        | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 4        | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 4        | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 4        | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 4        | 0.87          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 4        | 0.87          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 8        | 0.87          |
| (3,472) | 1:507:A:ILE:HA   | 1:510:A:TYR:HB2  | 10       | 0.87          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 19       | 0.87          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 19       | 0.87          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 3        | 0.87          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 3        | 0.87          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 3        | 0.87          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 3        | 0.87          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 3        | 0.87          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 3        | 0.87          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 15       | 0.87          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 15       | 0.87          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 1        | 0.86          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 1        | 0.86          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 5        | 0.86          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 5        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 3        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 9        | 0.86          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 9        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 9        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 9        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 9        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 9        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 9        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 9        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 9        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 9        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 9        | 0.86          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 9        | 0.86          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 19       | 0.86          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 19       | 0.86          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 6        | 0.86          |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 18       | 0.86          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 4        | 0.85          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 10       | 0.85          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 10       | 0.85          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 10       | 0.85          |
| (3,617) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HG   | 15       | 0.85          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 5        | 0.85          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 11       | 0.85          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 11       | 0.85          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 11       | 0.85          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 11       | 0.85          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 11       | 0.85          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 11       | 0.85          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 1        | 0.84          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 1        | 0.84          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 14       | 0.84          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 14       | 0.84          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 13       | 0.84          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 17       | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 5        | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 5        | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 5        | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 5        | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 5        | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 5        | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 5        | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 5        | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 5        | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 5        | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 5        | 0.84          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 5        | 0.84          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 17       | 0.84          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 3        | 0.84          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 3        | 0.84          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 17       | 0.84          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 17       | 0.84          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 20       | 0.84          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 20       | 0.84          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 4        | 0.84          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 4        | 0.84          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 4        | 0.84          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 4        | 0.84          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 4        | 0.84          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 4        | 0.84          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 8        | 0.84          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 8        | 0.84          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 8        | 0.84          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 8        | 0.84          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 16       | 0.84          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 16       | 0.84          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 16       | 0.84          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 16       | 0.84          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 16       | 0.84          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 16       | 0.84          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 16       | 0.84          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 16       | 0.84          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 16       | 0.84          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 16       | 0.84          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 16       | 0.84          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 16       | 0.84          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 7        | 0.83          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 7        | 0.83          |
| (3,899) | 1:554:A:THR:H    | 1:555:A:GLU:H    | 5        | 0.83          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 9        | 0.83          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 9        | 0.83          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 2        | 0.83          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 19       | 0.83          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 19       | 0.83          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 19       | 0.83          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 19       | 0.83          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 19       | 0.83          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 19       | 0.83          |
| (3,617) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HG   | 9        | 0.83          |
| (3,617) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HG   | 18       | 0.83          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 10       | 0.83          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 10       | 0.83          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 16       | 0.83          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 16       | 0.83          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 16       | 0.83          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 16       | 0.83          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 16       | 0.83          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 16       | 0.83          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 1        | 0.83          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 1        | 0.83          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 1        | 0.83          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 1        | 0.83          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2  | 19       | 0.82          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 19       | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 4        | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 4        | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 4        | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 4        | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 4        | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 4        | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 4        | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 4        | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 4        | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 4        | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 4        | 0.82          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 4        | 0.82          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 5        | 0.82          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 5        | 0.82          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 5        | 0.82          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 5        | 0.82          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 5        | 0.82          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 5        | 0.82          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 5        | 0.82          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 5        | 0.82          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 5        | 0.82          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 5        | 0.82          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 5        | 0.82          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 5        | 0.82          |
| (3,619) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HG   | 4        | 0.82          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 2        | 0.82          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 8        | 0.82          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 8        | 0.82          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 8        | 0.82          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 8        | 0.82          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 8        | 0.82          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 8        | 0.82          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 5        | 0.82          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 5        | 0.82          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 1        | 0.82          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 1        | 0.82          |
| (3,797) | 1:535:A:LYS:HB2  | 1:535:A:LYS:HE2  | 19       | 0.81          |
| (3,797) | 1:535:A:LYS:HB2  | 1:535:A:LYS:HE3  | 19       | 0.81          |
| (3,797) | 1:535:A:LYS:HB3  | 1:535:A:LYS:HE2  | 19       | 0.81          |
| (3,797) | 1:535:A:LYS:HB3  | 1:535:A:LYS:HE3  | 19       | 0.81          |
| (3,619) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HG   | 9        | 0.81          |
| (3,619) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HG   | 18       | 0.81          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 13       | 0.81          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 11       | 0.81          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2  | 3        | 0.8           |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 3        | 0.8           |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 9        | 0.8           |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 9        | 0.8           |
| (3,617) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HG   | 4        | 0.8           |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3  | 18       | 0.8           |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 10       | 0.8           |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 10       | 0.8           |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 10       | 0.8           |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 10       | 0.8           |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 10       | 0.8           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA  | 10       | 0.8           |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA  | 10       | 0.8           |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA  | 10       | 0.8           |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA  | 10       | 0.8           |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA  | 10       | 0.8           |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA  | 10       | 0.8           |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA  | 10       | 0.8           |
| (3,1)   | 1:445:A:ASN:HB2  | 1:446:A:ALA:H   | 19       | 0.8           |
| (3,895) | 1:552:A:ARG:HB2  | 1:553:A:GLY:H   | 5        | 0.79          |
| (3,895) | 1:552:A:ARG:HB3  | 1:553:A:GLY:H   | 5        | 0.79          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2 | 8        | 0.79          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3 | 8        | 0.79          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1 | 20       | 0.79          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1 | 20       | 0.79          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3 | 8        | 0.79          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3 | 10       | 0.79          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2 | 4        | 0.79          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2 | 4        | 0.79          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2 | 4        | 0.79          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2 | 4        | 0.79          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2 | 4        | 0.79          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2 | 4        | 0.79          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ  | 14       | 0.79          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ  | 14       | 0.79          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB  | 2        | 0.79          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB  | 2        | 0.79          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB  | 2        | 0.79          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB  | 2        | 0.79          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB  | 2        | 0.79          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB  | 2        | 0.79          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA  | 5        | 0.79          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA  | 5        | 0.79          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA  | 5        | 0.79          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA  | 5        | 0.79          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA  | 5        | 0.79          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA  | 5        | 0.79          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA  | 5        | 0.79          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA  | 5        | 0.79          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA  | 5        | 0.79          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA  | 5        | 0.79          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA  | 5        | 0.79          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA  | 5        | 0.79          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 10       | 0.78          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 10       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 17       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 17       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 17       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 17       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 17       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 17       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 17       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 17       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 17       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 17       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 17       | 0.78          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 17       | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 3        | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 3        | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 3        | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 3        | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 3        | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 3        | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 3        | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 3        | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 3        | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 3        | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 3        | 0.78          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 3        | 0.78          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 14       | 0.78          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 16       | 0.78          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 16       | 0.78          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 16       | 0.78          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 16       | 0.78          |
| (3,436) | 1:479:A:SER:HB2  | 1:506:A:VAL:HB   | 9        | 0.78          |
| (3,436) | 1:479:A:SER:HB3  | 1:506:A:VAL:HB   | 9        | 0.78          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 11       | 0.78          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 11       | 0.78          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 11       | 0.78          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 11       | 0.78          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 3        | 0.78          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 3        | 0.78          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 3        | 0.78          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 3        | 0.78          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 3        | 0.78          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 3        | 0.78          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 8        | 0.77          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 8        | 0.77          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 16       | 0.77          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 13       | 0.77          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 13       | 0.77          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 18       | 0.77          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 16       | 0.77          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 16       | 0.77          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 16       | 0.77          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 16       | 0.77          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 16       | 0.77          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 16       | 0.77          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 16       | 0.77          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 16       | 0.77          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 16       | 0.77          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 16       | 0.77          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 16       | 0.77          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 16       | 0.77          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 9        | 0.77          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 9        | 0.77          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 5        | 0.76          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 5        | 0.76          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 15       | 0.76          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 19       | 0.76          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 19       | 0.76          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 19       | 0.76          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 19       | 0.76          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 19       | 0.76          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 19       | 0.76          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 2        | 0.76          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 2        | 0.76          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 2        | 0.76          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 2        | 0.76          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 2        | 0.76          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 2        | 0.76          |
| (3,29)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HA   | 14       | 0.76          |
| (3,29)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HA   | 14       | 0.76          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 9        | 0.75          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 9        | 0.75          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG21 | 11       | 0.75          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG22 | 11       | 0.75          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG23 | 11       | 0.75          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 4        | 0.75          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 4        | 0.75          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 9        | 0.75          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 9        | 0.75          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 19       | 0.75          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 19       | 0.75          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 19       | 0.75          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 19       | 0.75          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 20       | 0.75          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 20       | 0.75          |
| (3,18)  | 1:451:A:PHE:HA   | 1:451:A:PHE:HD1  | 18       | 0.75          |
| (3,18)  | 1:451:A:PHE:HA   | 1:451:A:PHE:HD2  | 18       | 0.75          |
| (3,8)   | 1:447:A:THR:HG21 | 1:448:A:GLY:H    | 7        | 0.75          |
| (3,8)   | 1:447:A:THR:HG22 | 1:448:A:GLY:H    | 7        | 0.75          |
| (3,8)   | 1:447:A:THR:HG23 | 1:448:A:GLY:H    | 7        | 0.75          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD21 | 4        | 0.74          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD22 | 4        | 0.74          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 6        | 0.74          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 6        | 0.74          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 1        | 0.74          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 4        | 0.74          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 20       | 0.74          |
| (3,255) | 1:460:A:ILE:HD11 | 1:492:A:GLU:HA   | 1        | 0.74          |
| (3,255) | 1:460:A:ILE:HD12 | 1:492:A:GLU:HA   | 1        | 0.74          |
| (3,255) | 1:460:A:ILE:HD13 | 1:492:A:GLU:HA   | 1        | 0.74          |
| (3,255) | 1:460:A:ILE:HD11 | 1:492:A:GLU:HA   | 11       | 0.74          |
| (3,255) | 1:460:A:ILE:HD12 | 1:492:A:GLU:HA   | 11       | 0.74          |
| (3,255) | 1:460:A:ILE:HD13 | 1:492:A:GLU:HA   | 11       | 0.74          |
| (3,900) | 1:554:A:THR:HG21 | 1:555:A:GLU:H    | 3        | 0.73          |
| (3,900) | 1:554:A:THR:HG22 | 1:555:A:GLU:H    | 3        | 0.73          |
| (3,900) | 1:554:A:THR:HG23 | 1:555:A:GLU:H    | 3        | 0.73          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 11       | 0.73          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 7        | 0.73          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 7        | 0.73          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 10       | 0.73          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 7        | 0.73          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 7        | 0.73          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 7        | 0.73          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 7        | 0.73          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 7        | 0.73          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 7        | 0.73          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 20       | 0.73          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 20       | 0.73          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 6        | 0.73          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 6        | 0.73          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 6        | 0.73          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 6        | 0.73          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 4        | 0.73          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 4        | 0.73          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 4        | 0.73          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 4        | 0.73          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 4        | 0.73          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 4        | 0.73          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 4        | 0.73          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 4        | 0.73          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 4        | 0.73          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 4        | 0.73          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 4        | 0.73          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 4        | 0.73          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG21 | 10       | 0.72          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG22 | 10       | 0.72          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG23 | 10       | 0.72          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2  | 11       | 0.72          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 11       | 0.72          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 15       | 0.72          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 15       | 0.72          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 13       | 0.72          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 3        | 0.72          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 6        | 0.72          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 1        | 0.72          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 1        | 0.72          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 1        | 0.72          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 1        | 0.72          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 1        | 0.72          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 1        | 0.72          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 2        | 0.72          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 2        | 0.72          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 2        | 0.72          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 2        | 0.72          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 2        | 0.72          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 2        | 0.72          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 19       | 0.72          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 19       | 0.72          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 19       | 0.72          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 19       | 0.72          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 19       | 0.72          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 19       | 0.72          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 19       | 0.72          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 19       | 0.72          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 19       | 0.72          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 19       | 0.72          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 15       | 0.72          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 15       | 0.72          |
| (3,255) | 1:460:A:ILE:HD11 | 1:492:A:GLU:HA   | 12       | 0.72          |
| (3,255) | 1:460:A:ILE:HD12 | 1:492:A:GLU:HA   | 12       | 0.72          |
| (3,255) | 1:460:A:ILE:HD13 | 1:492:A:GLU:HA   | 12       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,33)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:H    | 11       | 0.72          |
| (3,29)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HA   | 5        | 0.72          |
| (3,29)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HA   | 5        | 0.72          |
| (3,911) | 1:558:A:ILE:HB   | 1:559:A:THR:H    | 8        | 0.71          |
| (3,893) | 1:552:A:ARG:H    | 1:552:A:ARG:HD2  | 9        | 0.71          |
| (3,893) | 1:552:A:ARG:H    | 1:552:A:ARG:HD3  | 9        | 0.71          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD2  | 14       | 0.71          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD3  | 14       | 0.71          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD2  | 19       | 0.71          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD3  | 19       | 0.71          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 13       | 0.71          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 13       | 0.71          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 17       | 0.71          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 17       | 0.71          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 12       | 0.71          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 12       | 0.71          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 18       | 0.71          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 10       | 0.71          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H   | 10       | 0.71          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H   | 1        | 0.71          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2 | 7        | 0.71          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3 | 7        | 0.71          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2 | 7        | 0.71          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3 | 7        | 0.71          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2 | 7        | 0.71          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3 | 7        | 0.71          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2 | 7        | 0.71          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3 | 7        | 0.71          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2 | 7        | 0.71          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3 | 7        | 0.71          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2 | 7        | 0.71          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3 | 7        | 0.71          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2 | 13       | 0.71          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2 | 13       | 0.71          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2 | 13       | 0.71          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3 | 13       | 0.71          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3 | 13       | 0.71          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3 | 13       | 0.71          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2 | 13       | 0.71          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2 | 13       | 0.71          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2 | 13       | 0.71          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3 | 13       | 0.71          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3 | 13       | 0.71          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3 | 13       | 0.71          |
| (3,13)  | 1:450:A:GLN:H    | 1:450:A:GLN:HG2 | 8        | 0.71          |
| (3,13)  | 1:450:A:GLN:H    | 1:450:A:GLN:HG3 | 8        | 0.71          |
| (3,896) | 1:553:A:GLY:H    | 1:554:A:THR:H   | 4        | 0.7           |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB  | 13       | 0.7           |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1 | 10       | 0.7           |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2 | 17       | 0.7           |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2 | 17       | 0.7           |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2 | 17       | 0.7           |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2 | 17       | 0.7           |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2 | 17       | 0.7           |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2 | 17       | 0.7           |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG  | 2        | 0.7           |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG  | 2        | 0.7           |
| (3,895) | 1:552:A:ARG:HB2  | 1:553:A:GLY:H   | 13       | 0.69          |
| (3,895) | 1:552:A:ARG:HB3  | 1:553:A:GLY:H   | 13       | 0.69          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2 | 9        | 0.69          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 9        | 0.69          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 7        | 0.69          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 19       | 0.69          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 11       | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 7        | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 7        | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 7        | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 7        | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 7        | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 7        | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 7        | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 7        | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 7        | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 7        | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 7        | 0.69          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 7        | 0.69          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 14       | 0.69          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 14       | 0.69          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 14       | 0.69          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 14       | 0.69          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 14       | 0.69          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 14       | 0.69          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 20       | 0.69          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 20       | 0.69          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 20       | 0.69          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 20       | 0.69          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 20       | 0.69          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 20       | 0.69          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 2        | 0.69          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 2        | 0.69          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 2        | 0.69          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 2        | 0.69          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 2        | 0.69          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 2        | 0.69          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 9        | 0.69          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 9        | 0.69          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 9        | 0.69          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 9        | 0.69          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 17       | 0.69          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 17       | 0.69          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 17       | 0.69          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 17       | 0.69          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2 | 10       | 0.69          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2 | 10       | 0.69          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2 | 10       | 0.69          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3 | 10       | 0.69          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3 | 10       | 0.69          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3 | 10       | 0.69          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2 | 10       | 0.69          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2 | 10       | 0.69          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2 | 10       | 0.69          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3 | 10       | 0.69          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3 | 10       | 0.69          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3 | 10       | 0.69          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2 | 9        | 0.69          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3 | 9        | 0.69          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2 | 9        | 0.69          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3 | 9        | 0.69          |
| (3,905) | 1:556:A:LYS:HG2  | 1:557:A:LEU:H   | 17       | 0.68          |
| (3,905) | 1:556:A:LYS:HG3  | 1:557:A:LEU:H   | 17       | 0.68          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG2 | 6        | 0.68          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG3 | 6        | 0.68          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD2 | 18       | 0.68          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD3 | 18       | 0.68          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H   | 4        | 0.68          |
| (3,619) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HG  | 15       | 0.68          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2 | 13       | 0.68          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2 | 13       | 0.68          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2 | 13       | 0.68          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3 | 13       | 0.68          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3 | 13       | 0.68          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3 | 13       | 0.68          |
| (3,581) | 1:474:A:THR:HB   | 1:519:A:TRP:HZ3 | 4        | 0.68          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2 | 9        | 0.68          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2 | 9        | 0.68          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2 | 9        | 0.68          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2 | 9        | 0.68          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2 | 9        | 0.68          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2 | 9        | 0.68          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1 | 16       | 0.68          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2 | 16       | 0.68          |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG2 | 1        | 0.68          |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG3 | 1        | 0.68          |
| (3,893) | 1:552:A:ARG:H    | 1:552:A:ARG:HD2 | 6        | 0.67          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (3,893) | 1:552:A:ARG:H    | 1:552:A:ARG:HD3 | 6        | 0.67          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2 | 20       | 0.67          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3 | 20       | 0.67          |
| (3,725) | 1:531:A:ARG:HD2  | 1:532:A:TYR:H   | 15       | 0.67          |
| (3,725) | 1:531:A:ARG:HD3  | 1:532:A:TYR:H   | 15       | 0.67          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H   | 14       | 0.67          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2 | 1        | 0.67          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2 | 1        | 0.67          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2 | 1        | 0.67          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2 | 1        | 0.67          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2 | 1        | 0.67          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2 | 1        | 0.67          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2 | 3        | 0.67          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2 | 3        | 0.67          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2 | 3        | 0.67          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2 | 3        | 0.67          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2 | 3        | 0.67          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2 | 3        | 0.67          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2 | 13       | 0.67          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2 | 13       | 0.67          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2 | 13       | 0.67          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2 | 13       | 0.67          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2 | 13       | 0.67          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2 | 13       | 0.67          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2 | 2        | 0.67          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3 | 2        | 0.67          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2 | 2        | 0.67          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3 | 2        | 0.67          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG2 | 2        | 0.66          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG3 | 2        | 0.66          |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2 | 18       | 0.66          |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2 | 18       | 0.66          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1 | 2        | 0.66          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2 | 11       | 0.66          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3 | 11       | 0.66          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2 | 11       | 0.66          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3 | 11       | 0.66          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2 | 11       | 0.66          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3 | 11       | 0.66          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2 | 16       | 0.66          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3 | 16       | 0.66          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2 | 16       | 0.66          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 16       | 0.66          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 16       | 0.66          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 16       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 14       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 14       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 14       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 14       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 14       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 14       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 14       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 14       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 14       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 14       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 14       | 0.66          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 14       | 0.66          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 6        | 0.66          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 6        | 0.66          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 6        | 0.66          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 6        | 0.66          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 6        | 0.66          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 6        | 0.66          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 11       | 0.66          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 9        | 0.66          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 9        | 0.66          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 9        | 0.66          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 9        | 0.66          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 19       | 0.66          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 19       | 0.66          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 19       | 0.66          |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 19       | 0.66          |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 19       | 0.66          |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 19       | 0.66          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG21 | 1        | 0.65          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG22 | 1        | 0.65          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG23 | 1        | 0.65          |
| (3,896) | 1:553:A:GLY:H    | 1:554:A:THR:H    | 19       | 0.65          |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2  | 5        | 0.65          |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2  | 5        | 0.65          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 6        | 0.65          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 20       | 0.65          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD11 | 3        | 0.65          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD12 | 3        | 0.65          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD13 | 3        | 0.65          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD21 | 3        | 0.65          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD22 | 3        | 0.65          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD23 | 3        | 0.65          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 12       | 0.65          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 12       | 0.65          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 12       | 0.65          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 12       | 0.65          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 12       | 0.65          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 12       | 0.65          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB2  | 11       | 0.65          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB3  | 11       | 0.65          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 19       | 0.65          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 13       | 0.65          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 13       | 0.65          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 4        | 0.65          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 4        | 0.65          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 4        | 0.65          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 4        | 0.65          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 16       | 0.65          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 16       | 0.65          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 16       | 0.65          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 16       | 0.65          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 16       | 0.65          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 16       | 0.65          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 16       | 0.65          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 16       | 0.65          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 16       | 0.65          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 16       | 0.65          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 16       | 0.65          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 16       | 0.65          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 1        | 0.65          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 1        | 0.65          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 1        | 0.65          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 1        | 0.65          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 1        | 0.65          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 1        | 0.65          |
| (3,911) | 1:558:A:ILE:HB   | 1:559:A:THR:H    | 17       | 0.64          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2  | 18       | 0.64          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 18       | 0.64          |
| (3,775) | 1:531:A:ARG:HA   | 1:534:A:GLN:HG2  | 9        | 0.64          |
| (3,775) | 1:531:A:ARG:HA   | 1:534:A:GLN:HG3  | 9        | 0.64          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 2        | 0.64          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 2        | 0.64          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 1        | 0.64          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 1        | 0.64          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 8        | 0.64          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 8        | 0.64          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 8        | 0.64          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 8        | 0.64          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 8        | 0.64          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 8        | 0.64          |
| (3,617) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HG   | 20       | 0.64          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 6        | 0.64          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 6        | 0.64          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 6        | 0.64          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 6        | 0.64          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 6        | 0.64          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 6        | 0.64          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 10       | 0.64          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 10       | 0.64          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 10       | 0.64          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 10       | 0.64          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 10       | 0.64          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 10       | 0.64          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD1  | 6        | 0.64          |
| (3,372) | 1:496:A:ARG:HA   | 1:497:A:PHE:HD2  | 6        | 0.64          |
| (3,913) | 1:558:A:ILE:HG21 | 1:559:A:THR:H    | 14       | 0.63          |
| (3,913) | 1:558:A:ILE:HG22 | 1:559:A:THR:H    | 14       | 0.63          |
| (3,913) | 1:558:A:ILE:HG23 | 1:559:A:THR:H    | 14       | 0.63          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 20       | 0.63          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 20       | 0.63          |
| (3,889) | 1:549:A:GLU:HG2  | 1:550:A:LYS:H    | 3        | 0.63          |
| (3,889) | 1:549:A:GLU:HG3  | 1:550:A:LYS:H    | 3        | 0.63          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 10       | 0.63          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 10       | 0.63          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 7        | 0.63          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 7        | 0.63          |
| (3,733) | 1:451:A:PHE:HE1  | 1:533:A:TRP:HD1  | 14       | 0.63          |
| (3,733) | 1:451:A:PHE:HE2  | 1:533:A:TRP:HD1  | 14       | 0.63          |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 12       | 0.63          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 12       | 0.63          |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 15       | 0.63          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 15       | 0.63          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 9        | 0.63          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 9        | 0.63          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 7        | 0.63          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 4        | 0.63          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 4        | 0.63          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 4        | 0.63          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 4        | 0.63          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 4        | 0.63          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 4        | 0.63          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 16       | 0.63          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 16       | 0.63          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 16       | 0.63          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 16       | 0.63          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 16       | 0.63          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 16       | 0.63          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 1        | 0.63          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 5        | 0.63          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 5        | 0.63          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 5        | 0.63          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 5        | 0.63          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 6        | 0.63          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 6        | 0.63          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 6        | 0.63          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 6        | 0.63          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 6        | 0.63          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 6        | 0.63          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 10       | 0.63          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 10       | 0.63          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 10       | 0.63          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 10       | 0.63          |
| (3,913) | 1:558:A:ILE:HG21 | 1:559:A:THR:H    | 11       | 0.62          |
| (3,913) | 1:558:A:ILE:HG22 | 1:559:A:THR:H    | 11       | 0.62          |
| (3,913) | 1:558:A:ILE:HG23 | 1:559:A:THR:H    | 11       | 0.62          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG21 | 1        | 0.62          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG22 | 1        | 0.62          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG23 | 1        | 0.62          |
| (3,895) | 1:552:A:ARG:HB2  | 1:553:A:GLY:H    | 19       | 0.62          |
| (3,895) | 1:552:A:ARG:HB3  | 1:553:A:GLY:H    | 19       | 0.62          |
| (3,746) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HZ2  | 11       | 0.62          |
| (3,746) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HZ2  | 11       | 0.62          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 20       | 0.62          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 13       | 0.62          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 13       | 0.62          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 8        | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 14       | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 14       | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 14       | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 14       | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 14       | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 14       | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 14       | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 14       | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 14       | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 14       | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 14       | 0.62          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 14       | 0.62          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 3        | 0.62          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 3        | 0.62          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 3        | 0.62          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 3        | 0.62          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 3        | 0.62          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 3        | 0.62          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 17       | 0.62          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 17       | 0.62          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 17       | 0.62          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 17       | 0.62          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 17       | 0.62          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 17       | 0.62          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 15       | 0.62          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 15       | 0.62          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 15       | 0.62          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 15       | 0.62          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 15       | 0.62          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 15       | 0.62          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 15       | 0.62          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 15       | 0.62          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 19       | 0.62          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 19       | 0.62          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 11       | 0.62          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 11       | 0.62          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 11       | 0.62          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 11       | 0.62          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 11       | 0.62          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 11       | 0.62          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 11       | 0.62          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 11       | 0.62          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 11       | 0.62          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 11       | 0.62          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 11       | 0.62          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 11       | 0.62          |
| (3,39)  | 1:455:A:VAL:H    | 1:456:A:ILE:H    | 18       | 0.62          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB2  | 8        | 0.62          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB2  | 8        | 0.62          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB3  | 8        | 0.62          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB3  | 8        | 0.62          |
| (3,913) | 1:558:A:ILE:HG21 | 1:559:A:THR:H    | 19       | 0.61          |
| (3,913) | 1:558:A:ILE:HG22 | 1:559:A:THR:H    | 19       | 0.61          |
| (3,913) | 1:558:A:ILE:HG23 | 1:559:A:THR:H    | 19       | 0.61          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG21 | 5        | 0.61          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG22 | 5        | 0.61          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG23 | 5        | 0.61          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG2  | 19       | 0.61          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG3  | 19       | 0.61          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 6        | 0.61          |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 1        | 0.61          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 1        | 0.61          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 2        | 0.61          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 2        | 0.61          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 16       | 0.61          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 18       | 0.61          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 8        | 0.61          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 8        | 0.61          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 8        | 0.61          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 8        | 0.61          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 8        | 0.61          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 8        | 0.61          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 10       | 0.61          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 10       | 0.61          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 10       | 0.61          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 10       | 0.61          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 10       | 0.61          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 10       | 0.61          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 11       | 0.61          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 11       | 0.61          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 11       | 0.61          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 11       | 0.61          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 11       | 0.61          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 11       | 0.61          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 15       | 0.61          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 15       | 0.61          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 15       | 0.61          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 15       | 0.61          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 15       | 0.61          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 15       | 0.61          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 14       | 0.61          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 14       | 0.61          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 14       | 0.61          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 14       | 0.61          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 14       | 0.61          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 14       | 0.61          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 16       | 0.61          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 6        | 0.61          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 17       | 0.61          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 17       | 0.61          |
| (3,39)  | 1:455:A:VAL:H    | 1:456:A:ILE:H    | 7        | 0.61          |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 7        | 0.61          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG2  | 10       | 0.6           |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG3  | 10       | 0.6           |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 11       | 0.6           |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 11       | 0.6           |
| (3,746) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HZ2  | 19       | 0.6           |
| (3,746) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HZ2  | 19       | 0.6           |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 6        | 0.6           |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 15       | 0.6           |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 4        | 0.6           |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 4        | 0.6           |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 5        | 0.6           |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 3        | 0.6           |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 3        | 0.6           |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 3        | 0.6           |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 3        | 0.6           |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 3        | 0.6           |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 3        | 0.6           |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 20       | 0.6           |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 20       | 0.6           |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 20       | 0.6           |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 20       | 0.6           |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 20       | 0.6           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 20       | 0.6           |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 5        | 0.6           |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 5        | 0.6           |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 5        | 0.6           |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 5        | 0.6           |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 5        | 0.6           |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 5        | 0.6           |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 9        | 0.6           |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 9        | 0.6           |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 9        | 0.6           |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 9        | 0.6           |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 9        | 0.6           |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 9        | 0.6           |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 12       | 0.6           |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 12       | 0.6           |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 12       | 0.6           |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 12       | 0.6           |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 12       | 0.6           |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 12       | 0.6           |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 8        | 0.6           |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 8        | 0.6           |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 8        | 0.6           |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 8        | 0.6           |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 2        | 0.6           |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 2        | 0.6           |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 2        | 0.6           |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 2        | 0.6           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 15       | 0.6           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 15       | 0.6           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 15       | 0.6           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 15       | 0.6           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 15       | 0.6           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 15       | 0.6           |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 2        | 0.59          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 2        | 0.59          |
| (3,883) | 1:548:A:ARG:HA   | 1:548:A:ARG:HD2  | 8        | 0.59          |
| (3,883) | 1:548:A:ARG:HA   | 1:548:A:ARG:HD3  | 8        | 0.59          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 1        | 0.59          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 1        | 0.59          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 12       | 0.59          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 4        | 0.59          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 4        | 0.59          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 4        | 0.59          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 4        | 0.59          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 4        | 0.59          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 4        | 0.59          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 6        | 0.59          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 6        | 0.59          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 18       | 0.59          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 18       | 0.59          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 18       | 0.59          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 18       | 0.59          |
| (3,859) | 1:539:A:ASP:HB3  | 1:540:A:ARG:HD2  | 18       | 0.58          |
| (3,859) | 1:539:A:ASP:HB3  | 1:540:A:ARG:HD3  | 18       | 0.58          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 20       | 0.58          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 20       | 0.58          |
| (3,751) | 1:496:A:ARG:HG2  | 1:533:A:TRP:HH2  | 15       | 0.58          |
| (3,751) | 1:496:A:ARG:HG3  | 1:533:A:TRP:HH2  | 15       | 0.58          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 16       | 0.58          |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 6        | 0.58          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 6        | 0.58          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 3        | 0.58          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 3        | 0.58          |
| (3,672) | 1:527:A:ASP:H    | 1:528:A:HIS:H    | 19       | 0.58          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 17       | 0.58          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 17       | 0.58          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 17       | 0.58          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 17       | 0.58          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 17       | 0.58          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 17       | 0.58          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 2        | 0.58          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 7        | 0.58          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 7        | 0.58          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 7        | 0.58          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 7        | 0.58          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 17       | 0.58          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 17       | 0.58          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 17       | 0.58          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 17       | 0.58          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 17       | 0.58          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 17       | 0.58          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 17       | 0.58          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 17       | 0.58          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 17       | 0.58          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 17       | 0.58          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 17       | 0.58          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 17       | 0.58          |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG2  | 6        | 0.58          |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG3  | 6        | 0.58          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 13       | 0.58          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 13       | 0.58          |
| (3,16)  | 1:450:A:GLN:H    | 1:451:A:PHE:HD1  | 16       | 0.58          |
| (3,16)  | 1:450:A:GLN:H    | 1:451:A:PHE:HD2  | 16       | 0.58          |
| (3,883) | 1:548:A:ARG:HA   | 1:548:A:ARG:HD2  | 3        | 0.57          |
| (3,883) | 1:548:A:ARG:HA   | 1:548:A:ARG:HD3  | 3        | 0.57          |
| (3,725) | 1:531:A:ARG:HD2  | 1:532:A:TYR:H    | 14       | 0.57          |
| (3,725) | 1:531:A:ARG:HD3  | 1:532:A:TYR:H    | 14       | 0.57          |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 16       | 0.57          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 16       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 5        | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 5        | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 5        | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 5        | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 5        | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 5        | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 10       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 10       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 10       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 10       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 10       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 10       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 13       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 13       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 13       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 13       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 13       | 0.57          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 13       | 0.57          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 8        | 0.57          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ   | 2        | 0.57          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ   | 2        | 0.57          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 18       | 0.57          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 18       | 0.57          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 18       | 0.57          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 18       | 0.57          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 18       | 0.57          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 18       | 0.57          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 18       | 0.57          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 18       | 0.57          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 18       | 0.57          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 18       | 0.57          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 18       | 0.57          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 18       | 0.57          |
| (3,101) | 1:465:A:LEU:HD11 | 1:467:A:GLY:H    | 9        | 0.57          |
| (3,101) | 1:465:A:LEU:HD12 | 1:467:A:GLY:H    | 9        | 0.57          |
| (3,101) | 1:465:A:LEU:HD13 | 1:467:A:GLY:H    | 9        | 0.57          |
| (3,101) | 1:465:A:LEU:HD21 | 1:467:A:GLY:H    | 9        | 0.57          |
| (3,101) | 1:465:A:LEU:HD22 | 1:467:A:GLY:H    | 9        | 0.57          |
| (3,101) | 1:465:A:LEU:HD23 | 1:467:A:GLY:H    | 9        | 0.57          |
| (3,39)  | 1:455:A:VAL:H    | 1:456:A:ILE:H    | 14       | 0.57          |
| (1,35)  | 1:500:A:PRO:O    | 1:504:A:GLN:H    | 14       | 0.57          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD21 | 17       | 0.56          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD22 | 17       | 0.56          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 5        | 0.56          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 5        | 0.56          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 9        | 0.56          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 4        | 0.56          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 4        | 0.56          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 16       | 0.56          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 16       | 0.56          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 6        | 0.56          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 6        | 0.56          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 6        | 0.56          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 6        | 0.56          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 6        | 0.56          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 6        | 0.56          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 9        | 0.56          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 9        | 0.56          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 9        | 0.56          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 9        | 0.56          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 9        | 0.56          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 9        | 0.56          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 13       | 0.56          |
| (3,571) | 1:465:A:LEU:HD11 | 1:519:A:TRP:HZ2  | 7        | 0.56          |
| (3,571) | 1:465:A:LEU:HD12 | 1:519:A:TRP:HZ2  | 7        | 0.56          |
| (3,571) | 1:465:A:LEU:HD13 | 1:519:A:TRP:HZ2  | 7        | 0.56          |
| (3,571) | 1:465:A:LEU:HD21 | 1:519:A:TRP:HZ2  | 7        | 0.56          |
| (3,571) | 1:465:A:LEU:HD22 | 1:519:A:TRP:HZ2  | 7        | 0.56          |
| (3,571) | 1:465:A:LEU:HD23 | 1:519:A:TRP:HZ2  | 7        | 0.56          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 6        | 0.56          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 6        | 0.56          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 6        | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 11       | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 11       | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 11       | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 11       | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 11       | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 11       | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 13       | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 13       | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 13       | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 13       | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 13       | 0.56          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 13       | 0.56          |
| (3,911) | 1:558:A:ILE:HB   | 1:559:A:THR:H    | 12       | 0.55          |
| (3,896) | 1:553:A:GLY:H    | 1:554:A:THR:H    | 2        | 0.55          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 11       | 0.55          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 11       | 0.55          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 11       | 0.55          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 3        | 0.55          |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 19       | 0.55          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 19       | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 4        | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 4        | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 4        | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 4        | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 4        | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 4        | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 19       | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 19       | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 19       | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 19       | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 19       | 0.55          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 19       | 0.55          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 6        | 0.55          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 13       | 0.55          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 13       | 0.55          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 13       | 0.55          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 19       | 0.55          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 19       | 0.55          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 15       | 0.55          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 15       | 0.55          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 15       | 0.55          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 15       | 0.55          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 16       | 0.55          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 16       | 0.55          |
| (3,39)  | 1:455:A:VAL:H    | 1:456:A:ILE:H    | 5        | 0.55          |
| (3,863) | 1:541:A:GLN:HA   | 1:541:A:GLN:HE21 | 5        | 0.54          |
| (3,863) | 1:541:A:GLN:HA   | 1:541:A:GLN:HE22 | 5        | 0.54          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 13       | 0.54          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 13       | 0.54          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 5        | 0.54          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 20       | 0.54          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 7        | 0.54          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 7        | 0.54          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 7        | 0.54          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 14       | 0.54          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 14       | 0.54          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 18       | 0.54          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 18       | 0.54          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 7        | 0.54          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 7        | 0.54          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 9        | 0.54          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 8        | 0.54          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 8        | 0.54          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 4        | 0.54          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 4        | 0.54          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 4        | 0.54          |
| (3,355) | 1:455:A:VAL:HG11 | 1:497:A:PHE:H    | 12       | 0.54          |
| (3,355) | 1:455:A:VAL:HG12 | 1:497:A:PHE:H    | 12       | 0.54          |
| (3,355) | 1:455:A:VAL:HG13 | 1:497:A:PHE:H    | 12       | 0.54          |
| (3,355) | 1:455:A:VAL:HG21 | 1:497:A:PHE:H    | 12       | 0.54          |
| (3,355) | 1:455:A:VAL:HG22 | 1:497:A:PHE:H    | 12       | 0.54          |
| (3,355) | 1:455:A:VAL:HG23 | 1:497:A:PHE:H    | 12       | 0.54          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 9        | 0.54          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 15       | 0.54          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 15       | 0.54          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 15       | 0.54          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 15       | 0.54          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 15       | 0.54          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 15       | 0.54          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 20       | 0.54          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 20       | 0.54          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 20       | 0.54          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 20       | 0.54          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 20       | 0.54          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 20       | 0.54          |
| (3,103) | 1:466:A:PRO:HD2  | 1:467:A:GLY:H    | 13       | 0.54          |
| (3,103) | 1:466:A:PRO:HD3  | 1:467:A:GLY:H    | 13       | 0.54          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 9        | 0.54          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 9        | 0.54          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 9        | 0.54          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 9        | 0.54          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 9        | 0.54          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 9        | 0.54          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE21 | 13       | 0.54          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE22 | 13       | 0.54          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG21 | 6        | 0.54          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG22 | 6        | 0.54          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG23 | 6        | 0.54          |
| (3,904) | 1:555:A:GLU:HB2  | 1:556:A:LYS:H    | 11       | 0.53          |
| (3,904) | 1:555:A:GLU:HB3  | 1:556:A:LYS:H    | 11       | 0.53          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG21 | 14       | 0.53          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG22 | 14       | 0.53          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG23 | 14       | 0.53          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 10       | 0.53          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 10       | 0.53          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 8        | 0.53          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 12       | 0.53          |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 10       | 0.53          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 10       | 0.53          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 15       | 0.53          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 15       | 0.53          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 2        | 0.53          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 12       | 0.53          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB2  | 18       | 0.53          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB2  | 18       | 0.53          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB2  | 18       | 0.53          |
| (3,586) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HB3  | 18       | 0.53          |
| (3,586) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HB3  | 18       | 0.53          |
| (3,586) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HB3  | 18       | 0.53          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 20       | 0.53          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 14       | 0.53          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 14       | 0.53          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 14       | 0.53          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 14       | 0.53          |
| (3,355) | 1:455:A:VAL:HG11 | 1:497:A:PHE:H    | 18       | 0.53          |
| (3,355) | 1:455:A:VAL:HG12 | 1:497:A:PHE:H    | 18       | 0.53          |
| (3,355) | 1:455:A:VAL:HG13 | 1:497:A:PHE:H    | 18       | 0.53          |
| (3,355) | 1:455:A:VAL:HG21 | 1:497:A:PHE:H    | 18       | 0.53          |
| (3,355) | 1:455:A:VAL:HG22 | 1:497:A:PHE:H    | 18       | 0.53          |
| (3,355) | 1:455:A:VAL:HG23 | 1:497:A:PHE:H    | 18       | 0.53          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 9        | 0.53          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 9        | 0.53          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 9        | 0.53          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 9        | 0.53          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 5        | 0.53          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 5        | 0.53          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 5        | 0.53          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 5        | 0.53          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 5        | 0.53          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 5        | 0.53          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 5        | 0.53          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 5        | 0.53          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 5        | 0.53          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 5        | 0.53          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 5        | 0.53          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 5        | 0.53          |
| (3,260) | 1:490:A:ASP:HB3  | 1:492:A:GLU:HG2  | 19       | 0.53          |
| (3,260) | 1:490:A:ASP:HB3  | 1:492:A:GLU:HG3  | 19       | 0.53          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 8        | 0.53          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 8        | 0.53          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 8        | 0.53          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 8        | 0.53          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 8        | 0.53          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 8        | 0.53          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 11       | 0.53          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 11       | 0.53          |
| (3,39)  | 1:455:A:VAL:H    | 1:456:A:ILE:H    | 12       | 0.53          |
| (1,37)  | 1:501:A:GLU:O    | 1:505:A:ALA:H    | 5        | 0.53          |
| (3,725) | 1:531:A:ARG:HD2  | 1:532:A:TYR:H    | 10       | 0.52          |
| (3,725) | 1:531:A:ARG:HD3  | 1:532:A:TYR:H    | 10       | 0.52          |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 17       | 0.52          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 17       | 0.52          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 11       | 0.52          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 11       | 0.52          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD11 | 4        | 0.52          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD12 | 4        | 0.52          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD13 | 4        | 0.52          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD21 | 4        | 0.52          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD22 | 4        | 0.52          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD23 | 4        | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 12       | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 12       | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 12       | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 12       | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 12       | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 12       | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 12       | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 12       | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 12       | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 12       | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 12       | 0.52          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 12       | 0.52          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 12       | 0.52          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 15       | 0.52          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 15       | 0.52          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 15       | 0.52          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 15       | 0.52          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 1        | 0.52          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 1        | 0.52          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 1        | 0.52          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 7        | 0.52          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 3        | 0.52          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 3        | 0.52          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 3        | 0.52          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 3        | 0.52          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 3        | 0.52          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3 | 3        | 0.52          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2 | 3        | 0.52          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3 | 3        | 0.52          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2 | 3        | 0.52          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3 | 3        | 0.52          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2 | 3        | 0.52          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3 | 3        | 0.52          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB  | 13       | 0.52          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB  | 13       | 0.52          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB  | 13       | 0.52          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB  | 13       | 0.52          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB  | 13       | 0.52          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB  | 13       | 0.52          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2 | 15       | 0.52          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3 | 15       | 0.52          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2 | 15       | 0.52          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3 | 15       | 0.52          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG  | 3        | 0.52          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG  | 3        | 0.52          |
| (3,904) | 1:555:A:GLU:HB2  | 1:556:A:LYS:H   | 8        | 0.51          |
| (3,904) | 1:555:A:GLU:HB3  | 1:556:A:LYS:H   | 8        | 0.51          |
| (3,891) | 1:550:A:LYS:HG2  | 1:551:A:LYS:H   | 1        | 0.51          |
| (3,891) | 1:550:A:LYS:HG3  | 1:551:A:LYS:H   | 1        | 0.51          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2 | 19       | 0.51          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2 | 19       | 0.51          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1 | 1        | 0.51          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA  | 5        | 0.51          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA  | 5        | 0.51          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1 | 3        | 0.51          |
| (3,493) | 1:511:A:THR:HG21 | 1:512:A:GLU:H   | 14       | 0.51          |
| (3,493) | 1:511:A:THR:HG22 | 1:512:A:GLU:H   | 14       | 0.51          |
| (3,493) | 1:511:A:THR:HG23 | 1:512:A:GLU:H   | 14       | 0.51          |
| (3,456) | 1:507:A:ILE:HD11 | 1:508:A:ASN:H   | 12       | 0.51          |
| (3,456) | 1:507:A:ILE:HD12 | 1:508:A:ASN:H   | 12       | 0.51          |
| (3,456) | 1:507:A:ILE:HD13 | 1:508:A:ASN:H   | 12       | 0.51          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2 | 2        | 0.51          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3 | 2        | 0.51          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2 | 5        | 0.51          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3 | 5        | 0.51          |
| (3,362) | 1:475:A:LEU:HB2  | 1:497:A:PHE:HZ  | 12       | 0.51          |
| (3,362) | 1:475:A:LEU:HB3  | 1:497:A:PHE:HZ  | 12       | 0.51          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2 | 5        | 0.51          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (3,279) | 1:486:A:LEU:HG  | 1:493:A:CYS:HB3  | 5        | 0.51          |
| (3,279) | 1:486:A:LEU:HG  | 1:493:A:CYS:HB2  | 5        | 0.51          |
| (3,279) | 1:486:A:LEU:HG  | 1:493:A:CYS:HB3  | 5        | 0.51          |
| (3,277) | 1:486:A:LEU:HA  | 1:493:A:CYS:HA   | 2        | 0.51          |
| (3,277) | 1:486:A:LEU:HA  | 1:493:A:CYS:HA   | 6        | 0.51          |
| (3,233) | 1:486:A:LEU:HG  | 1:487:A:LEU:H    | 1        | 0.51          |
| (3,129) | 1:470:A:GLN:HB2 | 1:471:A:VAL:H    | 4        | 0.51          |
| (3,129) | 1:470:A:GLN:HB3 | 1:471:A:VAL:H    | 4        | 0.51          |
| (3,129) | 1:470:A:GLN:HB2 | 1:471:A:VAL:H    | 19       | 0.51          |
| (3,129) | 1:470:A:GLN:HB3 | 1:471:A:VAL:H    | 19       | 0.51          |
| (3,94)  | 1:461:A:SER:HB2 | 1:465:A:LEU:HB2  | 8        | 0.51          |
| (3,94)  | 1:461:A:SER:HB2 | 1:465:A:LEU:HB3  | 8        | 0.51          |
| (3,94)  | 1:461:A:SER:HB3 | 1:465:A:LEU:HB2  | 8        | 0.51          |
| (3,94)  | 1:461:A:SER:HB3 | 1:465:A:LEU:HB3  | 8        | 0.51          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG11 | 10       | 0.51          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG12 | 10       | 0.51          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG13 | 10       | 0.51          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG21 | 10       | 0.51          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG22 | 10       | 0.51          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG23 | 10       | 0.51          |
| (3,859) | 1:539:A:ASP:HB3 | 1:540:A:ARG:HD2  | 3        | 0.5           |
| (3,859) | 1:539:A:ASP:HB3 | 1:540:A:ARG:HD3  | 3        | 0.5           |
| (3,748) | 1:496:A:ARG:HB2 | 1:533:A:TRP:HZ2  | 16       | 0.5           |
| (3,748) | 1:496:A:ARG:HB3 | 1:533:A:TRP:HZ2  | 16       | 0.5           |
| (3,734) | 1:456:A:ILE:H   | 1:533:A:TRP:HE1  | 3        | 0.5           |
| (3,734) | 1:456:A:ILE:H   | 1:533:A:TRP:HE1  | 16       | 0.5           |
| (3,649) | 1:494:A:HIS:HD2 | 1:524:A:LEU:HD11 | 10       | 0.5           |
| (3,649) | 1:494:A:HIS:HD2 | 1:524:A:LEU:HD12 | 10       | 0.5           |
| (3,649) | 1:494:A:HIS:HD2 | 1:524:A:LEU:HD13 | 10       | 0.5           |
| (3,649) | 1:494:A:HIS:HD2 | 1:524:A:LEU:HD21 | 10       | 0.5           |
| (3,649) | 1:494:A:HIS:HD2 | 1:524:A:LEU:HD22 | 10       | 0.5           |
| (3,649) | 1:494:A:HIS:HD2 | 1:524:A:LEU:HD23 | 10       | 0.5           |
| (3,626) | 1:521:A:LEU:H   | 1:521:A:LEU:HD11 | 18       | 0.5           |
| (3,626) | 1:521:A:LEU:H   | 1:521:A:LEU:HD12 | 18       | 0.5           |
| (3,626) | 1:521:A:LEU:H   | 1:521:A:LEU:HD13 | 18       | 0.5           |
| (3,626) | 1:521:A:LEU:H   | 1:521:A:LEU:HD21 | 18       | 0.5           |
| (3,626) | 1:521:A:LEU:H   | 1:521:A:LEU:HD22 | 18       | 0.5           |
| (3,626) | 1:521:A:LEU:H   | 1:521:A:LEU:HD23 | 18       | 0.5           |
| (3,602) | 1:519:A:TRP:HD1 | 1:520:A:LYS:H    | 1        | 0.5           |
| (3,602) | 1:519:A:TRP:HD1 | 1:520:A:LYS:H    | 15       | 0.5           |
| (3,487) | 1:511:A:THR:H   | 1:511:A:THR:HG21 | 16       | 0.5           |
| (3,487) | 1:511:A:THR:H   | 1:511:A:THR:HG22 | 16       | 0.5           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 16       | 0.5           |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB2  | 17       | 0.5           |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB2  | 17       | 0.5           |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB2  | 17       | 0.5           |
| (3,334) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HB3  | 17       | 0.5           |
| (3,334) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HB3  | 17       | 0.5           |
| (3,334) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HB3  | 17       | 0.5           |
| (3,303) | 1:459:A:ILE:HG12 | 1:494:A:HIS:HA   | 11       | 0.5           |
| (3,303) | 1:459:A:ILE:HG13 | 1:494:A:HIS:HA   | 11       | 0.5           |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 4        | 0.5           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 1        | 0.5           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 1        | 0.5           |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 1        | 0.5           |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 1        | 0.5           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 1        | 0.5           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 1        | 0.5           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 1        | 0.5           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 1        | 0.5           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 1        | 0.5           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 1        | 0.5           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 1        | 0.5           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 1        | 0.5           |
| (3,233) | 1:486:A:LEU:HG   | 1:487:A:LEU:H    | 20       | 0.5           |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 2        | 0.5           |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 2        | 0.5           |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 7        | 0.5           |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 7        | 0.5           |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 9        | 0.5           |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 9        | 0.5           |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 15       | 0.5           |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 15       | 0.5           |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 20       | 0.5           |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 20       | 0.5           |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 20       | 0.5           |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 20       | 0.5           |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB2  | 18       | 0.5           |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB2  | 18       | 0.5           |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB3  | 18       | 0.5           |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB3  | 18       | 0.5           |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 19       | 0.5           |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 19       | 0.5           |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 19       | 0.5           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 19       | 0.5           |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 19       | 0.5           |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 19       | 0.5           |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD2  | 5        | 0.49          |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD3  | 5        | 0.49          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD2  | 16       | 0.49          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD3  | 16       | 0.49          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 2        | 0.49          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 4        | 0.49          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 12       | 0.49          |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 11       | 0.49          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 11       | 0.49          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 12       | 0.49          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 12       | 0.49          |
| (3,653) | 1:524:A:LEU:H    | 1:524:A:LEU:HG   | 9        | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 1        | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 1        | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 1        | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 1        | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 1        | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 1        | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 16       | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 16       | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 16       | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 16       | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 16       | 0.49          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 16       | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 1        | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 1        | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 1        | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 1        | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 1        | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 1        | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 1        | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 1        | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 1        | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 1        | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 1        | 0.49          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 1        | 0.49          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 14       | 0.49          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 14       | 0.49          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 2        | 0.49          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 2        | 0.49          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 2        | 0.49          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 2        | 0.49          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 15       | 0.49          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 15       | 0.49          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 15       | 0.49          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 1        | 0.49          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 1        | 0.49          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 3        | 0.49          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 3        | 0.49          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 16       | 0.49          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 16       | 0.49          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 2        | 0.49          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 2        | 0.49          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 2        | 0.49          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 2        | 0.49          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 2        | 0.49          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 2        | 0.49          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE21 | 6        | 0.49          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE22 | 6        | 0.49          |
| (3,8)   | 1:447:A:THR:HG21 | 1:448:A:GLY:H    | 12       | 0.49          |
| (3,8)   | 1:447:A:THR:HG22 | 1:448:A:GLY:H    | 12       | 0.49          |
| (3,8)   | 1:447:A:THR:HG23 | 1:448:A:GLY:H    | 12       | 0.49          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 6        | 0.48          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 6        | 0.48          |
| (3,888) | 1:549:A:GLU:HB2  | 1:550:A:LYS:H    | 3        | 0.48          |
| (3,888) | 1:549:A:GLU:HB3  | 1:550:A:LYS:H    | 3        | 0.48          |
| (3,775) | 1:531:A:ARG:HA   | 1:534:A:GLN:HG2  | 15       | 0.48          |
| (3,775) | 1:531:A:ARG:HA   | 1:534:A:GLN:HG3  | 15       | 0.48          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG2  | 20       | 0.48          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG3  | 20       | 0.48          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG2  | 20       | 0.48          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG3  | 20       | 0.48          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 18       | 0.48          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 19       | 0.48          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 19       | 0.48          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 2        | 0.48          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 2        | 0.48          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 2        | 0.48          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 2        | 0.48          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 2        | 0.48          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 2        | 0.48          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 2        | 0.48          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 2        | 0.48          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 2        | 0.48          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 2        | 0.48          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 2        | 0.48          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 2        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 7        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 7        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 7        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 7        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 7        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 7        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 7        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 7        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 7        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 7        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 7        | 0.48          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 7        | 0.48          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 7        | 0.48          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 20       | 0.48          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 4        | 0.48          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 6        | 0.48          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 6        | 0.48          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 6        | 0.48          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 6        | 0.48          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 19       | 0.48          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 19       | 0.48          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 19       | 0.48          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 19       | 0.48          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 14       | 0.48          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 14       | 0.48          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 14       | 0.48          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 14       | 0.48          |
| (3,233) | 1:486:A:LEU:HG   | 1:487:A:LEU:H    | 11       | 0.48          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 12       | 0.48          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 12       | 0.48          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 12       | 0.48          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 12       | 0.48          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 12       | 0.48          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 12       | 0.48          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 5        | 0.48          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 5        | 0.48          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 1        | 0.48          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 1        | 0.48          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 20       | 0.48          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 20       | 0.48          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 20       | 0.48          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 20       | 0.48          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 20       | 0.48          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 20       | 0.48          |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG2  | 20       | 0.47          |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG3  | 20       | 0.47          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG21 | 9        | 0.47          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG22 | 9        | 0.47          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG23 | 9        | 0.47          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG2  | 3        | 0.47          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG3  | 3        | 0.47          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG2  | 3        | 0.47          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG3  | 3        | 0.47          |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2  | 14       | 0.47          |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2  | 14       | 0.47          |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 18       | 0.47          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 18       | 0.47          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 20       | 0.47          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 20       | 0.47          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD11 | 15       | 0.47          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD12 | 15       | 0.47          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD13 | 15       | 0.47          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD21 | 15       | 0.47          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD22 | 15       | 0.47          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD23 | 15       | 0.47          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 8        | 0.47          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 8        | 0.47          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 19       | 0.47          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 19       | 0.47          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 18       | 0.47          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 18       | 0.47          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 18       | 0.47          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 18       | 0.47          |
| (3,436) | 1:479:A:SER:HB2  | 1:506:A:VAL:HB   | 3        | 0.47          |
| (3,436) | 1:479:A:SER:HB3  | 1:506:A:VAL:HB   | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 3        | 0.47          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 3        | 0.47          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 20       | 0.47          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 20       | 0.47          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 20       | 0.47          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 20       | 0.47          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 20       | 0.47          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 20       | 0.47          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 20       | 0.47          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 20       | 0.47          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 20       | 0.47          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 20       | 0.47          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 20       | 0.47          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 20       | 0.47          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 12       | 0.47          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 12       | 0.47          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 18       | 0.47          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 18       | 0.47          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 20       | 0.47          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 20       | 0.47          |
| (3,103) | 1:466:A:PRO:HD2  | 1:467:A:GLY:H    | 15       | 0.47          |
| (3,103) | 1:466:A:PRO:HD3  | 1:467:A:GLY:H    | 15       | 0.47          |
| (3,882) | 1:548:A:ARG:H    | 1:548:A:ARG:HG2  | 18       | 0.46          |
| (3,882) | 1:548:A:ARG:H    | 1:548:A:ARG:HG3  | 18       | 0.46          |
| (3,874) | 1:545:A:ASN:H    | 1:546:A:GLN:H    | 18       | 0.46          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 4        | 0.46          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 4        | 0.46          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 10       | 0.46          |
| (3,731) | 1:451:A:PHE:HD1  | 1:533:A:TRP:HB3  | 14       | 0.46          |
| (3,731) | 1:451:A:PHE:HD2  | 1:533:A:TRP:HB3  | 14       | 0.46          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 17       | 0.46          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 17       | 0.46          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 13       | 0.46          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 13       | 0.46          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD11 | 9        | 0.46          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD12 | 9        | 0.46          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD13 | 9        | 0.46          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD21 | 9        | 0.46          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD22 | 9        | 0.46          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD23 | 9        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 2        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 2        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 2        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 2        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 2        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 2        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 2        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 2        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 2        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 2        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 2        | 0.46          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 2        | 0.46          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 11       | 0.46          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 2        | 0.46          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 2        | 0.46          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 6        | 0.46          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 6        | 0.46          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 7        | 0.46          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 7        | 0.46          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 13       | 0.46          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 13       | 0.46          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 15       | 0.46          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 15       | 0.46          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 3        | 0.46          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 11       | 0.46          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 11       | 0.46          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 11       | 0.46          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 11       | 0.46          |
| (3,355) | 1:455:A:VAL:HG11 | 1:497:A:PHE:H    | 7        | 0.46          |
| (3,355) | 1:455:A:VAL:HG12 | 1:497:A:PHE:H    | 7        | 0.46          |
| (3,355) | 1:455:A:VAL:HG13 | 1:497:A:PHE:H    | 7        | 0.46          |
| (3,355) | 1:455:A:VAL:HG21 | 1:497:A:PHE:H    | 7        | 0.46          |
| (3,355) | 1:455:A:VAL:HG22 | 1:497:A:PHE:H    | 7        | 0.46          |
| (3,355) | 1:455:A:VAL:HG23 | 1:497:A:PHE:H    | 7        | 0.46          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 18       | 0.46          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 8        | 0.46          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 8        | 0.46          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 17       | 0.46          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 17       | 0.46          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 17       | 0.46          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 17       | 0.46          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 18       | 0.46          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 18       | 0.46          |
| (3,6)   | 1:446:A:ALA:HB1  | 1:447:A:THR:H    | 11       | 0.46          |
| (3,6)   | 1:446:A:ALA:HB2  | 1:447:A:THR:H    | 11       | 0.46          |
| (3,6)   | 1:446:A:ALA:HB3  | 1:447:A:THR:H    | 11       | 0.46          |
| (1,35)  | 1:500:A:PRO:O    | 1:504:A:GLN:H    | 5        | 0.46          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG21 | 7        | 0.45          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG22 | 7        | 0.45          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG23 | 7        | 0.45          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG21 | 18       | 0.45          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG22 | 18       | 0.45          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG23 | 18       | 0.45          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD2  | 10       | 0.45          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD3  | 10       | 0.45          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD2  | 10       | 0.45          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD3  | 10       | 0.45          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 20       | 0.45          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 20       | 0.45          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 8        | 0.45          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 8        | 0.45          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 8        | 0.45          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 8        | 0.45          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 8        | 0.45          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 8        | 0.45          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 5        | 0.45          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 5        | 0.45          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 11       | 0.45          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 11       | 0.45          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 17       | 0.45          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 17       | 0.45          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB2  | 3        | 0.45          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB3  | 3        | 0.45          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 5        | 0.45          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 5        | 0.45          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 11       | 0.45          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 11       | 0.45          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 11       | 0.45          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 11       | 0.45          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB2  | 10       | 0.45          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB3  | 10       | 0.45          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB2  | 10       | 0.45          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB3  | 10       | 0.45          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 10       | 0.45          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 10       | 0.45          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 13       | 0.45          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 13       | 0.45          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 16       | 0.45          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 16       | 0.45          |
| (3,355) | 1:455:A:VAL:HG11 | 1:497:A:PHE:H    | 5        | 0.45          |
| (3,355) | 1:455:A:VAL:HG12 | 1:497:A:PHE:H    | 5        | 0.45          |
| (3,355) | 1:455:A:VAL:HG13 | 1:497:A:PHE:H    | 5        | 0.45          |
| (3,355) | 1:455:A:VAL:HG21 | 1:497:A:PHE:H    | 5        | 0.45          |
| (3,355) | 1:455:A:VAL:HG22 | 1:497:A:PHE:H    | 5        | 0.45          |
| (3,355) | 1:455:A:VAL:HG23 | 1:497:A:PHE:H    | 5        | 0.45          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 1        | 0.45          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 12       | 0.45          |
| (3,255) | 1:460:A:ILE:HD11 | 1:492:A:GLU:HA   | 7        | 0.45          |
| (3,255) | 1:460:A:ILE:HD12 | 1:492:A:GLU:HA   | 7        | 0.45          |
| (3,255) | 1:460:A:ILE:HD13 | 1:492:A:GLU:HA   | 7        | 0.45          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 10       | 0.45          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 10       | 0.45          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 13       | 0.45          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 13       | 0.45          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 1        | 0.45          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 1        | 0.45          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 1        | 0.45          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 1        | 0.45          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 1        | 0.45          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 1        | 0.45          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 17       | 0.44          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 17       | 0.44          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG2  | 12       | 0.44          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG3  | 12       | 0.44          |
| (3,883) | 1:548:A:ARG:HA   | 1:548:A:ARG:HD2  | 5        | 0.44          |
| (3,883) | 1:548:A:ARG:HA   | 1:548:A:ARG:HD3  | 5        | 0.44          |
| (3,793) | 1:535:A:LYS:H    | 1:535:A:LYS:HG2  | 14       | 0.44          |
| (3,793) | 1:535:A:LYS:H    | 1:535:A:LYS:HG3  | 14       | 0.44          |
| (3,793) | 1:535:A:LYS:H    | 1:535:A:LYS:HG2  | 19       | 0.44          |
| (3,793) | 1:535:A:LYS:H    | 1:535:A:LYS:HG3  | 19       | 0.44          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 19       | 0.44          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 19       | 0.44          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 8        | 0.44          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 19       | 0.44          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 1        | 0.44          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 1        | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 19       | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 19       | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 19       | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 19       | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 19       | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 19       | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 19       | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 19       | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 19       | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 19       | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 19       | 0.44          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 19       | 0.44          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 3        | 0.44          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 3        | 0.44          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 4        | 0.44          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 4        | 0.44          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 3        | 0.44          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 3        | 0.44          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 8        | 0.44          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 8        | 0.44          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 9        | 0.44          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 9        | 0.44          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 9        | 0.44          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 9        | 0.44          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 6        | 0.44          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 6        | 0.44          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 14       | 0.44          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 14       | 0.44          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 17       | 0.44          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 17       | 0.44          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 17       | 0.44          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 17       | 0.44          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 17       | 0.44          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 17       | 0.44          |
| (3,8)   | 1:447:A:THR:HG21 | 1:448:A:GLY:H    | 3        | 0.44          |
| (3,8)   | 1:447:A:THR:HG22 | 1:448:A:GLY:H    | 3        | 0.44          |
| (3,8)   | 1:447:A:THR:HG23 | 1:448:A:GLY:H    | 3        | 0.44          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 14       | 0.43          |
| (3,708) | 1:530:A:GLN:HG2  | 1:531:A:ARG:H    | 7        | 0.43          |
| (3,708) | 1:530:A:GLN:HG3  | 1:531:A:ARG:H    | 7        | 0.43          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 8        | 0.43          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 8        | 0.43          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 11       | 0.43          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 11       | 0.43          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 11       | 0.43          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 11       | 0.43          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 11       | 0.43          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 11       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 19       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 19       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 19       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 19       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 19       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 19       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 19       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 19       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 19       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 19       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 19       | 0.43          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 19       | 0.43          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 14       | 0.43          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 1        | 0.43          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 10       | 0.43          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 10       | 0.43          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 5        | 0.43          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 5        | 0.43          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 5        | 0.43          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 19       | 0.43          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 19       | 0.43          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 19       | 0.43          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 16       | 0.43          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 10       | 0.43          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 10       | 0.43          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 10       | 0.43          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 10       | 0.43          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 12       | 0.43          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 12       | 0.43          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 12       | 0.43          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 12       | 0.43          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 11       | 0.43          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 11       | 0.43          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 11       | 0.43          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 20       | 0.43          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 20       | 0.43          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 20       | 0.43          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 5        | 0.43          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 5        | 0.43          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 5        | 0.43          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 5        | 0.43          |
| (3,297) | 1:458:A:LYS:HD2  | 1:494:A:HIS:HD2  | 18       | 0.43          |
| (3,297) | 1:458:A:LYS:HD3  | 1:494:A:HIS:HD2  | 18       | 0.43          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 7        | 0.43          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 14       | 0.43          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 20       | 0.43          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 16       | 0.43          |
| (3,233) | 1:486:A:LEU:HG   | 1:487:A:LEU:H    | 12       | 0.43          |
| (3,129) | 1:470:A:GLN:HB2  | 1:471:A:VAL:H    | 11       | 0.43          |
| (3,129) | 1:470:A:GLN:HB3  | 1:471:A:VAL:H    | 11       | 0.43          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 17       | 0.43          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 17       | 0.43          |
| (3,29)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HA   | 12       | 0.43          |
| (3,29)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HA   | 12       | 0.43          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 18       | 0.43          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 18       | 0.43          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 18       | 0.43          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 18       | 0.43          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 18       | 0.43          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 18       | 0.43          |
| (3,882) | 1:548:A:ARG:H    | 1:548:A:ARG:HG2  | 6        | 0.42          |
| (3,882) | 1:548:A:ARG:H    | 1:548:A:ARG:HG3  | 6        | 0.42          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,877) | 1:546:A:GLN:HG2  | 1:547:A:PRO:HD2  | 13       | 0.42          |
| (3,877) | 1:546:A:GLN:HG2  | 1:547:A:PRO:HD3  | 13       | 0.42          |
| (3,877) | 1:546:A:GLN:HG3  | 1:547:A:PRO:HD2  | 13       | 0.42          |
| (3,877) | 1:546:A:GLN:HG3  | 1:547:A:PRO:HD3  | 13       | 0.42          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 3        | 0.42          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 3        | 0.42          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 11       | 0.42          |
| (3,731) | 1:451:A:PHE:HD1  | 1:533:A:TRP:HB3  | 5        | 0.42          |
| (3,731) | 1:451:A:PHE:HD2  | 1:533:A:TRP:HB3  | 5        | 0.42          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 15       | 0.42          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 15       | 0.42          |
| (3,617) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HG   | 17       | 0.42          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 19       | 0.42          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 3        | 0.42          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 3        | 0.42          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 3        | 0.42          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 13       | 0.42          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 13       | 0.42          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 13       | 0.42          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 17       | 0.42          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 17       | 0.42          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 17       | 0.42          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB2  | 20       | 0.42          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB3  | 20       | 0.42          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 17       | 0.42          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 17       | 0.42          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 17       | 0.42          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 17       | 0.42          |
| (3,436) | 1:479:A:SER:HB2  | 1:506:A:VAL:HB   | 5        | 0.42          |
| (3,436) | 1:479:A:SER:HB3  | 1:506:A:VAL:HB   | 5        | 0.42          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB2  | 13       | 0.42          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB3  | 13       | 0.42          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB2  | 13       | 0.42          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB3  | 13       | 0.42          |
| (3,260) | 1:490:A:ASP:HB3  | 1:492:A:GLU:HG2  | 10       | 0.42          |
| (3,260) | 1:490:A:ASP:HB3  | 1:492:A:GLU:HG3  | 10       | 0.42          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 1        | 0.42          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 1        | 0.42          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 1        | 0.42          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 1        | 0.42          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 1        | 0.42          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 1        | 0.42          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 1        | 0.42          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 1        | 0.42          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 1        | 0.42          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 1        | 0.42          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 1        | 0.42          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 1        | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 2        | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 2        | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 2        | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 2        | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 2        | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 2        | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 11       | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 11       | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 11       | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 11       | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 11       | 0.42          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 11       | 0.42          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 11       | 0.42          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 11       | 0.42          |
| (3,29)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HA   | 10       | 0.42          |
| (3,29)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HA   | 10       | 0.42          |
| (3,29)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HA   | 15       | 0.42          |
| (3,29)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HA   | 15       | 0.42          |
| (3,6)   | 1:446:A:ALA:HB1  | 1:447:A:THR:H    | 1        | 0.42          |
| (3,6)   | 1:446:A:ALA:HB2  | 1:447:A:THR:H    | 1        | 0.42          |
| (3,6)   | 1:446:A:ALA:HB3  | 1:447:A:THR:H    | 1        | 0.42          |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 14       | 0.42          |
| (3,911) | 1:558:A:ILE:HB   | 1:559:A:THR:H    | 20       | 0.41          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 12       | 0.41          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 12       | 0.41          |
| (3,895) | 1:552:A:ARG:HB2  | 1:553:A:GLY:H    | 3        | 0.41          |
| (3,895) | 1:552:A:ARG:HB3  | 1:553:A:GLY:H    | 3        | 0.41          |
| (3,891) | 1:550:A:LYS:HG2  | 1:551:A:LYS:H    | 14       | 0.41          |
| (3,891) | 1:550:A:LYS:HG3  | 1:551:A:LYS:H    | 14       | 0.41          |
| (3,874) | 1:545:A:ASN:H    | 1:546:A:GLN:H    | 14       | 0.41          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG2  | 7        | 0.41          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG3  | 7        | 0.41          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG2  | 7        | 0.41          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG3  | 7        | 0.41          |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2  | 3        | 0.41          |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2  | 3        | 0.41          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 6        | 0.41          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 6        | 0.41          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 17       | 0.41          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 17       | 0.41          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 19       | 0.41          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 19       | 0.41          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 5        | 0.41          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 9        | 0.41          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 16       | 0.41          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 16       | 0.41          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 4        | 0.41          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 4        | 0.41          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 4        | 0.41          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 10       | 0.41          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 10       | 0.41          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 10       | 0.41          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 12       | 0.41          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 12       | 0.41          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 12       | 0.41          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 18       | 0.41          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 18       | 0.41          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 18       | 0.41          |
| (3,493) | 1:511:A:THR:HG21 | 1:512:A:GLU:H    | 13       | 0.41          |
| (3,493) | 1:511:A:THR:HG22 | 1:512:A:GLU:H    | 13       | 0.41          |
| (3,493) | 1:511:A:THR:HG23 | 1:512:A:GLU:H    | 13       | 0.41          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 14       | 0.41          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 14       | 0.41          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 14       | 0.41          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 15       | 0.41          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 15       | 0.41          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 16       | 0.41          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 9        | 0.41          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 9        | 0.41          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 9        | 0.41          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 9        | 0.41          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 9        | 0.41          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 9        | 0.41          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 9        | 0.41          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 9        | 0.41          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 9        | 0.41          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 9        | 0.41          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 9        | 0.41          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 9        | 0.41          |
| (3,103) | 1:466:A:PRO:HD2  | 1:467:A:GLY:H    | 2        | 0.41          |
| (3,103) | 1:466:A:PRO:HD3  | 1:467:A:GLY:H    | 2        | 0.41          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 18       | 0.41          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 18       | 0.41          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 18       | 0.41          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 18       | 0.41          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 4        | 0.41          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 4        | 0.41          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 8        | 0.41          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 8        | 0.41          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE21 | 2        | 0.41          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE22 | 2        | 0.41          |
| (3,6)   | 1:446:A:ALA:HB1  | 1:447:A:THR:H    | 19       | 0.41          |
| (3,6)   | 1:446:A:ALA:HB2  | 1:447:A:THR:H    | 19       | 0.41          |
| (3,6)   | 1:446:A:ALA:HB3  | 1:447:A:THR:H    | 19       | 0.41          |
| (1,37)  | 1:501:A:GLU:O    | 1:505:A:ALA:H    | 18       | 0.41          |
| (3,899) | 1:554:A:THR:H    | 1:555:A:GLU:H    | 20       | 0.4           |
| (3,858) | 1:536:A:ILE:HG21 | 1:540:A:ARG:HD2  | 3        | 0.4           |
| (3,858) | 1:536:A:ILE:HG21 | 1:540:A:ARG:HD3  | 3        | 0.4           |
| (3,858) | 1:536:A:ILE:HG22 | 1:540:A:ARG:HD2  | 3        | 0.4           |
| (3,858) | 1:536:A:ILE:HG22 | 1:540:A:ARG:HD3  | 3        | 0.4           |
| (3,858) | 1:536:A:ILE:HG23 | 1:540:A:ARG:HD2  | 3        | 0.4           |
| (3,858) | 1:536:A:ILE:HG23 | 1:540:A:ARG:HD3  | 3        | 0.4           |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 12       | 0.4           |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2  | 16       | 0.4           |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2  | 16       | 0.4           |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD11 | 8        | 0.4           |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD12 | 8        | 0.4           |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD13 | 8        | 0.4           |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD21 | 8        | 0.4           |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD22 | 8        | 0.4           |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD23 | 8        | 0.4           |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 7        | 0.4           |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 10       | 0.4           |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 8        | 0.4           |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 8        | 0.4           |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 20       | 0.4           |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 20       | 0.4           |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 8        | 0.4           |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 8        | 0.4           |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 8        | 0.4           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 11       | 0.4           |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 11       | 0.4           |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 11       | 0.4           |
| (3,493) | 1:511:A:THR:HG21 | 1:512:A:GLU:H    | 4        | 0.4           |
| (3,493) | 1:511:A:THR:HG22 | 1:512:A:GLU:H    | 4        | 0.4           |
| (3,493) | 1:511:A:THR:HG23 | 1:512:A:GLU:H    | 4        | 0.4           |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE1  | 9        | 0.4           |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE2  | 9        | 0.4           |
| (3,456) | 1:507:A:ILE:HD11 | 1:508:A:ASN:H    | 19       | 0.4           |
| (3,456) | 1:507:A:ILE:HD12 | 1:508:A:ASN:H    | 19       | 0.4           |
| (3,456) | 1:507:A:ILE:HD13 | 1:508:A:ASN:H    | 19       | 0.4           |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 15       | 0.4           |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 15       | 0.4           |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 15       | 0.4           |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 15       | 0.4           |
| (3,436) | 1:479:A:SER:HB2  | 1:506:A:VAL:HB   | 13       | 0.4           |
| (3,436) | 1:479:A:SER:HB3  | 1:506:A:VAL:HB   | 13       | 0.4           |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 10       | 0.4           |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 10       | 0.4           |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 5        | 0.4           |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 5        | 0.4           |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 16       | 0.4           |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 16       | 0.4           |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 18       | 0.4           |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 18       | 0.4           |
| (3,303) | 1:459:A:ILE:HG12 | 1:494:A:HIS:HA   | 14       | 0.4           |
| (3,303) | 1:459:A:ILE:HG13 | 1:494:A:HIS:HA   | 14       | 0.4           |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 5        | 0.4           |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 5        | 0.4           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 20       | 0.4           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 20       | 0.4           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 20       | 0.4           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 20       | 0.4           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 20       | 0.4           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 20       | 0.4           |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB2  | 3        | 0.4           |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB2  | 3        | 0.4           |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB3  | 3        | 0.4           |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB3  | 3        | 0.4           |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 1        | 0.39          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 1        | 0.39          |
| (3,894) | 1:552:A:ARG:HA   | 1:552:A:ARG:HD2  | 10       | 0.39          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,894) | 1:552:A:ARG:HA   | 1:552:A:ARG:HD3  | 10       | 0.39          |
| (3,858) | 1:536:A:ILE:HG21 | 1:540:A:ARG:HD2  | 4        | 0.39          |
| (3,858) | 1:536:A:ILE:HG21 | 1:540:A:ARG:HD3  | 4        | 0.39          |
| (3,858) | 1:536:A:ILE:HG22 | 1:540:A:ARG:HD2  | 4        | 0.39          |
| (3,858) | 1:536:A:ILE:HG22 | 1:540:A:ARG:HD3  | 4        | 0.39          |
| (3,858) | 1:536:A:ILE:HG23 | 1:540:A:ARG:HD2  | 4        | 0.39          |
| (3,858) | 1:536:A:ILE:HG23 | 1:540:A:ARG:HD3  | 4        | 0.39          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG2  | 14       | 0.39          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG3  | 14       | 0.39          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG2  | 14       | 0.39          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG3  | 14       | 0.39          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 18       | 0.39          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 6        | 0.39          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 12       | 0.39          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 19       | 0.39          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 18       | 0.39          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 18       | 0.39          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 6        | 0.39          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 6        | 0.39          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 6        | 0.39          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB2  | 4        | 0.39          |
| (3,544) | 1:514:A:ASN:HD21 | 1:518:A:CYS:HB3  | 4        | 0.39          |
| (3,493) | 1:511:A:THR:HG21 | 1:512:A:GLU:H    | 19       | 0.39          |
| (3,493) | 1:511:A:THR:HG22 | 1:512:A:GLU:H    | 19       | 0.39          |
| (3,493) | 1:511:A:THR:HG23 | 1:512:A:GLU:H    | 19       | 0.39          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 10       | 0.39          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 10       | 0.39          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 10       | 0.39          |
| (3,456) | 1:507:A:ILE:HD11 | 1:508:A:ASN:H    | 1        | 0.39          |
| (3,456) | 1:507:A:ILE:HD12 | 1:508:A:ASN:H    | 1        | 0.39          |
| (3,456) | 1:507:A:ILE:HD13 | 1:508:A:ASN:H    | 1        | 0.39          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 3        | 0.39          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 3        | 0.39          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 20       | 0.39          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 20       | 0.39          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD2  | 5        | 0.39          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD2  | 5        | 0.39          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD2  | 5        | 0.39          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD3  | 5        | 0.39          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD3  | 5        | 0.39          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD3  | 5        | 0.39          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 1        | 0.39          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 1        | 0.39          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 1        | 0.39          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 1        | 0.39          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 7        | 0.39          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 7        | 0.39          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 7        | 0.39          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 7        | 0.39          |
| (3,260) | 1:490:A:ASP:HB3  | 1:492:A:GLU:HG2  | 11       | 0.39          |
| (3,260) | 1:490:A:ASP:HB3  | 1:492:A:GLU:HG3  | 11       | 0.39          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 16       | 0.39          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 16       | 0.39          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 16       | 0.39          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 16       | 0.39          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 16       | 0.39          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 16       | 0.39          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 3        | 0.39          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 3        | 0.39          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 6        | 0.39          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 6        | 0.39          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 13       | 0.39          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 13       | 0.39          |
| (1,37)  | 1:501:A:GLU:O    | 1:505:A:ALA:H    | 14       | 0.39          |
| (3,912) | 1:558:A:ILE:HD11 | 1:559:A:THR:H    | 7        | 0.38          |
| (3,912) | 1:558:A:ILE:HD12 | 1:559:A:THR:H    | 7        | 0.38          |
| (3,912) | 1:558:A:ILE:HD13 | 1:559:A:THR:H    | 7        | 0.38          |
| (3,890) | 1:550:A:LYS:H    | 1:550:A:LYS:HG2  | 6        | 0.38          |
| (3,890) | 1:550:A:LYS:H    | 1:550:A:LYS:HG3  | 6        | 0.38          |
| (3,888) | 1:549:A:GLU:HB2  | 1:550:A:LYS:H    | 6        | 0.38          |
| (3,888) | 1:549:A:GLU:HB3  | 1:550:A:LYS:H    | 6        | 0.38          |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2  | 7        | 0.38          |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2  | 7        | 0.38          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 17       | 0.38          |
| (3,706) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 14       | 0.38          |
| (3,706) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 14       | 0.38          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 18       | 0.38          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 18       | 0.38          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 18       | 0.38          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 18       | 0.38          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 18       | 0.38          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 18       | 0.38          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 10       | 0.38          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 4        | 0.38          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 5        | 0.38          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 8        | 0.38          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 14       | 0.38          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 17       | 0.38          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 18       | 0.38          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 20       | 0.38          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 9        | 0.38          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 9        | 0.38          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 9        | 0.38          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 14       | 0.38          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 14       | 0.38          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 14       | 0.38          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 16       | 0.38          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 16       | 0.38          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 16       | 0.38          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 7        | 0.38          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 19       | 0.38          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 19       | 0.38          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 19       | 0.38          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 11       | 0.38          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 11       | 0.38          |
| (3,233) | 1:486:A:LEU:HG   | 1:487:A:LEU:H    | 7        | 0.38          |
| (3,233) | 1:486:A:LEU:HG   | 1:487:A:LEU:H    | 14       | 0.38          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD11 | 10       | 0.38          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD12 | 10       | 0.38          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD13 | 10       | 0.38          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD21 | 10       | 0.38          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD22 | 10       | 0.38          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD23 | 10       | 0.38          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 8        | 0.38          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 8        | 0.38          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB2  | 10       | 0.38          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB2  | 10       | 0.38          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB3  | 10       | 0.38          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB3  | 10       | 0.38          |
| (3,9)   | 1:448:A:GLY:H    | 1:449:A:PRO:HD2  | 17       | 0.38          |
| (3,9)   | 1:448:A:GLY:H    | 1:449:A:PRO:HD3  | 17       | 0.38          |
| (3,899) | 1:554:A:THR:H    | 1:555:A:GLU:H    | 14       | 0.37          |
| (3,896) | 1:553:A:GLY:H    | 1:554:A:THR:H    | 7        | 0.37          |
| (3,889) | 1:549:A:GLU:HG2  | 1:550:A:LYS:H    | 9        | 0.37          |
| (3,889) | 1:549:A:GLU:HG3  | 1:550:A:LYS:H    | 9        | 0.37          |
| (3,863) | 1:541:A:GLN:HA   | 1:541:A:GLN:HE21 | 4        | 0.37          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,863) | 1:541:A:GLN:HA   | 1:541:A:GLN:HE22 | 4        | 0.37          |
| (3,786) | 1:532:A:TYR:HE1  | 1:535:A:LYS:HD2  | 14       | 0.37          |
| (3,786) | 1:532:A:TYR:HE1  | 1:535:A:LYS:HD3  | 14       | 0.37          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD2  | 5        | 0.37          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD3  | 5        | 0.37          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 14       | 0.37          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 14       | 0.37          |
| (3,746) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HZ2  | 10       | 0.37          |
| (3,746) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HZ2  | 10       | 0.37          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 15       | 0.37          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 15       | 0.37          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 15       | 0.37          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 15       | 0.37          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 15       | 0.37          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 15       | 0.37          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 15       | 0.37          |
| (3,640) | 1:523:A:ILE:H    | 1:523:A:ILE:HD11 | 18       | 0.37          |
| (3,640) | 1:523:A:ILE:H    | 1:523:A:ILE:HD12 | 18       | 0.37          |
| (3,640) | 1:523:A:ILE:H    | 1:523:A:ILE:HD13 | 18       | 0.37          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 3        | 0.37          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 3        | 0.37          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 3        | 0.37          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 3        | 0.37          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 3        | 0.37          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 3        | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 12       | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 12       | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 12       | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 12       | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 12       | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 12       | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 12       | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 12       | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 12       | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 12       | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 12       | 0.37          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 12       | 0.37          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 11       | 0.37          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 13       | 0.37          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 16       | 0.37          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 17       | 0.37          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 2        | 0.37          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 2        | 0.37          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 2        | 0.37          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 15       | 0.37          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 15       | 0.37          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 15       | 0.37          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB2  | 6        | 0.37          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB3  | 6        | 0.37          |
| (3,496) | 1:513:A:ILE:H    | 1:513:A:ILE:HD11 | 18       | 0.37          |
| (3,496) | 1:513:A:ILE:H    | 1:513:A:ILE:HD12 | 18       | 0.37          |
| (3,496) | 1:513:A:ILE:H    | 1:513:A:ILE:HD13 | 18       | 0.37          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 6        | 0.37          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD2  | 7        | 0.37          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD2  | 7        | 0.37          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD2  | 7        | 0.37          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD3  | 7        | 0.37          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD3  | 7        | 0.37          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD3  | 7        | 0.37          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 16       | 0.37          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 16       | 0.37          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 16       | 0.37          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 16       | 0.37          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 13       | 0.37          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 13       | 0.37          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 13       | 0.37          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 2        | 0.37          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 4        | 0.37          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 4        | 0.37          |
| (3,29)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HA   | 4        | 0.37          |
| (3,29)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HA   | 4        | 0.37          |
| (3,29)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HA   | 7        | 0.37          |
| (3,29)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HA   | 7        | 0.37          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,29)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HA   | 11       | 0.37          |
| (3,29)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HA   | 11       | 0.37          |
| (1,39)  | 1:502:A:ASP:O    | 1:506:A:VAL:H    | 18       | 0.37          |
| (1,36)  | 1:500:A:PRO:O    | 1:504:A:GLN:N    | 14       | 0.37          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 5        | 0.36          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 4        | 0.36          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 4        | 0.36          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 5        | 0.36          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 5        | 0.36          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 16       | 0.36          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 16       | 0.36          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 17       | 0.36          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 9        | 0.36          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 9        | 0.36          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 2        | 0.36          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 14       | 0.36          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 14       | 0.36          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 20       | 0.36          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 20       | 0.36          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 20       | 0.36          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 13       | 0.36          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 3        | 0.36          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 3        | 0.36          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 3        | 0.36          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 3        | 0.36          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE2  | 17       | 0.36          |
| (3,524) | 1:516:A:LYS:HB2  | 1:516:A:LYS:HE3  | 17       | 0.36          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE2  | 17       | 0.36          |
| (3,524) | 1:516:A:LYS:HB3  | 1:516:A:LYS:HE3  | 17       | 0.36          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 8        | 0.36          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 8        | 0.36          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 8        | 0.36          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 8        | 0.36          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 14       | 0.36          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 14       | 0.36          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 18       | 0.36          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 12       | 0.36          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 12       | 0.36          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 12       | 0.36          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 12       | 0.36          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 13       | 0.36          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 13       | 0.36          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 13       | 0.36          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 13       | 0.36          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 19       | 0.36          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 19       | 0.36          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 20       | 0.36          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 20       | 0.36          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 20       | 0.36          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 20       | 0.36          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 20       | 0.36          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 20       | 0.36          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 20       | 0.36          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 20       | 0.36          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 20       | 0.36          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 20       | 0.36          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 20       | 0.36          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 20       | 0.36          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD11 | 8        | 0.36          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD12 | 8        | 0.36          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD13 | 8        | 0.36          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD21 | 8        | 0.36          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD22 | 8        | 0.36          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD23 | 8        | 0.36          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 19       | 0.36          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 19       | 0.36          |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 15       | 0.36          |
| (1,39)  | 1:502:A:ASP:O    | 1:506:A:VAL:H    | 5        | 0.36          |
| (3,884) | 1:548:A:ARG:HD2  | 1:549:A:GLU:H    | 11       | 0.35          |
| (3,884) | 1:548:A:ARG:HD3  | 1:549:A:GLU:H    | 11       | 0.35          |
| (3,840) | 1:534:A:GLN:HA   | 1:537:A:LEU:HD11 | 4        | 0.35          |
| (3,840) | 1:534:A:GLN:HA   | 1:537:A:LEU:HD12 | 4        | 0.35          |
| (3,840) | 1:534:A:GLN:HA   | 1:537:A:LEU:HD13 | 4        | 0.35          |
| (3,840) | 1:534:A:GLN:HA   | 1:537:A:LEU:HD21 | 4        | 0.35          |
| (3,840) | 1:534:A:GLN:HA   | 1:537:A:LEU:HD22 | 4        | 0.35          |
| (3,840) | 1:534:A:GLN:HA   | 1:537:A:LEU:HD23 | 4        | 0.35          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG21 | 20       | 0.35          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG22 | 20       | 0.35          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG23 | 20       | 0.35          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 9        | 0.35          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 9        | 0.35          |
| (3,786) | 1:532:A:TYR:HE1  | 1:535:A:LYS:HD2  | 19       | 0.35          |
| (3,786) | 1:532:A:TYR:HE1  | 1:535:A:LYS:HD3  | 19       | 0.35          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 3        | 0.35          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 3        | 0.35          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 17       | 0.35          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 17       | 0.35          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 2        | 0.35          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 2        | 0.35          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 8        | 0.35          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 8        | 0.35          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 12       | 0.35          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 12       | 0.35          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 12       | 0.35          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 12       | 0.35          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 12       | 0.35          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 12       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 16       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 16       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 16       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 16       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 16       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 16       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 16       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 16       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 16       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 16       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 16       | 0.35          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 16       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 14       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 14       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 14       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 14       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 14       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 14       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 14       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 14       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 14       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 14       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 14       | 0.35          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 14       | 0.35          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 3        | 0.35          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 8        | 0.35          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 9        | 0.35          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 3        | 0.35          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 12       | 0.35          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 12       | 0.35          |
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 1        | 0.35          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 1        | 0.35          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 1        | 0.35          |
| (3,513) | 1:515:A:LYS:H    | 1:515:A:LYS:HD2  | 15       | 0.35          |
| (3,513) | 1:515:A:LYS:H    | 1:515:A:LYS:HD3  | 15       | 0.35          |
| (3,457) | 1:507:A:ILE:HD11 | 1:508:A:ASN:HD22 | 12       | 0.35          |
| (3,457) | 1:507:A:ILE:HD12 | 1:508:A:ASN:HD22 | 12       | 0.35          |
| (3,457) | 1:507:A:ILE:HD13 | 1:508:A:ASN:HD22 | 12       | 0.35          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 13       | 0.35          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 13       | 0.35          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 13       | 0.35          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 13       | 0.35          |
| (3,355) | 1:455:A:VAL:HG11 | 1:497:A:PHE:H    | 14       | 0.35          |
| (3,355) | 1:455:A:VAL:HG12 | 1:497:A:PHE:H    | 14       | 0.35          |
| (3,355) | 1:455:A:VAL:HG13 | 1:497:A:PHE:H    | 14       | 0.35          |
| (3,355) | 1:455:A:VAL:HG21 | 1:497:A:PHE:H    | 14       | 0.35          |
| (3,355) | 1:455:A:VAL:HG22 | 1:497:A:PHE:H    | 14       | 0.35          |
| (3,355) | 1:455:A:VAL:HG23 | 1:497:A:PHE:H    | 14       | 0.35          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 4        | 0.35          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 4        | 0.35          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD2  | 19       | 0.35          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD2  | 19       | 0.35          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD2  | 19       | 0.35          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD3  | 19       | 0.35          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD3  | 19       | 0.35          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD3  | 19       | 0.35          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB1  | 15       | 0.35          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB2  | 15       | 0.35          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB3  | 15       | 0.35          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB2  | 19       | 0.35          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB3  | 19       | 0.35          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB2  | 19       | 0.35          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB3  | 19       | 0.35          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 7        | 0.35          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 7        | 0.35          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 14       | 0.35          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 14       | 0.35          |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD2  | 2        | 0.35          |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD3  | 2        | 0.35          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB2  | 11       | 0.35          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB2  | 11       | 0.35          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB3  | 11       | 0.35          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB3  | 11       | 0.35          |
| (3,6)   | 1:446:A:ALA:HB1  | 1:447:A:THR:H    | 5        | 0.35          |
| (3,6)   | 1:446:A:ALA:HB2  | 1:447:A:THR:H    | 5        | 0.35          |
| (3,6)   | 1:446:A:ALA:HB3  | 1:447:A:THR:H    | 5        | 0.35          |
| (3,913) | 1:558:A:ILE:HG21 | 1:559:A:THR:H    | 8        | 0.34          |
| (3,913) | 1:558:A:ILE:HG22 | 1:559:A:THR:H    | 8        | 0.34          |
| (3,913) | 1:558:A:ILE:HG23 | 1:559:A:THR:H    | 8        | 0.34          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD11 | 7        | 0.34          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD12 | 7        | 0.34          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD13 | 7        | 0.34          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 8        | 0.34          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 8        | 0.34          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 14       | 0.34          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 5        | 0.34          |
| (3,734) | 1:456:A:ILE:H    | 1:533:A:TRP:HE1  | 13       | 0.34          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 12       | 0.34          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 12       | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 6        | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 6        | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 6        | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 6        | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 6        | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 6        | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 6        | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 6        | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 6        | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 6        | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 6        | 0.34          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 6        | 0.34          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 4        | 0.34          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB2  | 9        | 0.34          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB3  | 9        | 0.34          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB1  | 3        | 0.34          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB2  | 3        | 0.34          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB3  | 3        | 0.34          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 12       | 0.34          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 12       | 0.34          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 12       | 0.34          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 12       | 0.34          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 1        | 0.34          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 1        | 0.34          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 1        | 0.34          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 1        | 0.34          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 1        | 0.34          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 1        | 0.34          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 1        | 0.34          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 1        | 0.34          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 1        | 0.34          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 1        | 0.34          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 1        | 0.34          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 1        | 0.34          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 6        | 0.34          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 14       | 0.34          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 13       | 0.33          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 13       | 0.33          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD11 | 8        | 0.33          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD12 | 8        | 0.33          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD13 | 8        | 0.33          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 1        | 0.33          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 1        | 0.33          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 6        | 0.33          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 6        | 0.33          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 3        | 0.33          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 3        | 0.33          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD11 | 5        | 0.33          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD12 | 5        | 0.33          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD13 | 5        | 0.33          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD21 | 5        | 0.33          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD22 | 5        | 0.33          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD23 | 5        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 2        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 2        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 2        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 2        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 2        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 2        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 2        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 2        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 2        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 2        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 2        | 0.33          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 2        | 0.33          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 17       | 0.33          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 17       | 0.33          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 17       | 0.33          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 8        | 0.33          |
| (3,456) | 1:507:A:ILE:HD11 | 1:508:A:ASN:H    | 18       | 0.33          |
| (3,456) | 1:507:A:ILE:HD12 | 1:508:A:ASN:H    | 18       | 0.33          |
| (3,456) | 1:507:A:ILE:HD13 | 1:508:A:ASN:H    | 18       | 0.33          |
| (3,410) | 1:501:A:GLU:HG2  | 1:502:A:ASP:H    | 10       | 0.33          |
| (3,410) | 1:501:A:GLU:HG3  | 1:502:A:ASP:H    | 10       | 0.33          |
| (3,410) | 1:501:A:GLU:HG2  | 1:502:A:ASP:H    | 11       | 0.33          |
| (3,410) | 1:501:A:GLU:HG3  | 1:502:A:ASP:H    | 11       | 0.33          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB2  | 1        | 0.33          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB3  | 1        | 0.33          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB2  | 1        | 0.33          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB3  | 1        | 0.33          |
| (3,297) | 1:458:A:LYS:HD2  | 1:494:A:HIS:HD2  | 20       | 0.33          |
| (3,297) | 1:458:A:LYS:HD3  | 1:494:A:HIS:HD2  | 20       | 0.33          |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG2  | 15       | 0.33          |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG3  | 15       | 0.33          |
| (3,233) | 1:486:A:LEU:HG   | 1:487:A:LEU:H    | 9        | 0.33          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD11 | 13       | 0.33          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD12 | 13       | 0.33          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD13 | 13       | 0.33          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD21 | 13       | 0.33          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD22 | 13       | 0.33          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD23 | 13       | 0.33          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD11 | 1        | 0.33          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD12 | 1        | 0.33          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD13 | 1        | 0.33          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD21 | 1        | 0.33          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD22 | 1        | 0.33          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD23 | 1        | 0.33          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 6        | 0.33          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 6        | 0.33          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 6        | 0.33          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 6        | 0.33          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 6        | 0.33          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 6        | 0.33          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 10       | 0.33          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 10       | 0.33          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 7        | 0.33          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 7        | 0.33          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 7        | 0.33          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 7        | 0.33          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 7        | 0.33          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 7        | 0.33          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 5        | 0.33          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 5        | 0.33          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 16       | 0.33          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 16       | 0.33          |
| (1,39)  | 1:502:A:ASP:O    | 1:506:A:VAL:H    | 12       | 0.33          |
| (3,820) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HB   | 18       | 0.32          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG2  | 17       | 0.32          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG3  | 17       | 0.32          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG2  | 17       | 0.32          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG3  | 17       | 0.32          |
| (3,735) | 1:456:A:ILE:HG12 | 1:533:A:TRP:HE1  | 7        | 0.32          |
| (3,720) | 1:524:A:LEU:HD11 | 1:532:A:TYR:HD2  | 14       | 0.32          |
| (3,720) | 1:524:A:LEU:HD12 | 1:532:A:TYR:HD2  | 14       | 0.32          |
| (3,720) | 1:524:A:LEU:HD13 | 1:532:A:TYR:HD2  | 14       | 0.32          |
| (3,720) | 1:524:A:LEU:HD21 | 1:532:A:TYR:HD2  | 14       | 0.32          |
| (3,720) | 1:524:A:LEU:HD22 | 1:532:A:TYR:HD2  | 14       | 0.32          |
| (3,720) | 1:524:A:LEU:HD23 | 1:532:A:TYR:HD2  | 14       | 0.32          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,706) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 18       | 0.32          |
| (3,706) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 18       | 0.32          |
| (3,703) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 11       | 0.32          |
| (3,703) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 11       | 0.32          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD11 | 7        | 0.32          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD12 | 7        | 0.32          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD13 | 7        | 0.32          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD21 | 7        | 0.32          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD22 | 7        | 0.32          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD23 | 7        | 0.32          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 13       | 0.32          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 13       | 0.32          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 13       | 0.32          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 13       | 0.32          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 13       | 0.32          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 13       | 0.32          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 20       | 0.32          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 20       | 0.32          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 20       | 0.32          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 20       | 0.32          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 20       | 0.32          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 20       | 0.32          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 6        | 0.32          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 6        | 0.32          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 6        | 0.32          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 6        | 0.32          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 6        | 0.32          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 6        | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 13       | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 13       | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 13       | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 13       | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 13       | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 13       | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 13       | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 13       | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 13       | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 13       | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 13       | 0.32          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 13       | 0.32          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 4        | 0.32          |
| (3,566) | 1:462:A:THR:H    | 1:519:A:TRP:HE1  | 15       | 0.32          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,551) | 1:459:A:ILE:HG21 | 1:519:A:TRP:HA   | 7        | 0.32          |
| (3,551) | 1:459:A:ILE:HG22 | 1:519:A:TRP:HA   | 7        | 0.32          |
| (3,551) | 1:459:A:ILE:HG23 | 1:519:A:TRP:HA   | 7        | 0.32          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 3        | 0.32          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 13       | 0.32          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 13       | 0.32          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 13       | 0.32          |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD21 | 7        | 0.32          |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD21 | 7        | 0.32          |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD22 | 7        | 0.32          |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD22 | 7        | 0.32          |
| (3,457) | 1:507:A:ILE:HD11 | 1:508:A:ASN:HD22 | 11       | 0.32          |
| (3,457) | 1:507:A:ILE:HD12 | 1:508:A:ASN:HD22 | 11       | 0.32          |
| (3,457) | 1:507:A:ILE:HD13 | 1:508:A:ASN:HD22 | 11       | 0.32          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB2  | 19       | 0.32          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB3  | 19       | 0.32          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB2  | 19       | 0.32          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB3  | 19       | 0.32          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 11       | 0.32          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 11       | 0.32          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 4        | 0.32          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 4        | 0.32          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 13       | 0.32          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 17       | 0.32          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 17       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD11 | 15       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD12 | 15       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD13 | 15       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD21 | 15       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD22 | 15       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD23 | 15       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD11 | 17       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD12 | 17       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD13 | 17       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD21 | 17       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD22 | 17       | 0.32          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD23 | 17       | 0.32          |
| (3,183) | 1:478:A:ILE:HB   | 1:479:A:SER:HB2  | 19       | 0.32          |
| (3,183) | 1:478:A:ILE:HB   | 1:479:A:SER:HB3  | 19       | 0.32          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 19       | 0.32          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 19       | 0.32          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2  | 1        | 0.31          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 1        | 0.31          |
| (3,882) | 1:548:A:ARG:H    | 1:548:A:ARG:HG2  | 14       | 0.31          |
| (3,882) | 1:548:A:ARG:H    | 1:548:A:ARG:HG3  | 14       | 0.31          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD2  | 11       | 0.31          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD3  | 11       | 0.31          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD2  | 11       | 0.31          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD3  | 11       | 0.31          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 2        | 0.31          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 2        | 0.31          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 11       | 0.31          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 11       | 0.31          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 18       | 0.31          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 18       | 0.31          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 17       | 0.31          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 17       | 0.31          |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2  | 13       | 0.31          |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2  | 13       | 0.31          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD11 | 15       | 0.31          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD12 | 15       | 0.31          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD13 | 15       | 0.31          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD21 | 15       | 0.31          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD22 | 15       | 0.31          |
| (3,627) | 1:521:A:LEU:HA   | 1:521:A:LEU:HD23 | 15       | 0.31          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD11 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD12 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD13 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD21 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD22 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD23 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD11 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD12 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD13 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD21 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD22 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD23 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD11 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD12 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD13 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD21 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD22 | 17       | 0.31          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD23 | 17       | 0.31          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 6        | 0.31          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB2  | 16       | 0.31          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB3  | 16       | 0.31          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 4        | 0.31          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 4        | 0.31          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 4        | 0.31          |
| (3,493) | 1:511:A:THR:HG21 | 1:512:A:GLU:H    | 16       | 0.31          |
| (3,493) | 1:511:A:THR:HG22 | 1:512:A:GLU:H    | 16       | 0.31          |
| (3,493) | 1:511:A:THR:HG23 | 1:512:A:GLU:H    | 16       | 0.31          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB2  | 7        | 0.31          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB3  | 7        | 0.31          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB2  | 7        | 0.31          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB3  | 7        | 0.31          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 3        | 0.31          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 3        | 0.31          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 14       | 0.31          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 14       | 0.31          |
| (3,325) | 1:485:A:ASP:H    | 1:495:A:ALA:HA   | 11       | 0.31          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 10       | 0.31          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 10       | 0.31          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 10       | 0.31          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 10       | 0.31          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 10       | 0.31          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 10       | 0.31          |
| (3,17)  | 1:450:A:GLN:HA   | 1:451:A:PHE:HD1  | 17       | 0.31          |
| (3,17)  | 1:450:A:GLN:HA   | 1:451:A:PHE:HD2  | 17       | 0.31          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE21 | 8        | 0.31          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE22 | 8        | 0.31          |
| (1,43)  | 1:504:A:GLN:O    | 1:508:A:ASN:H    | 7        | 0.31          |
| (1,35)  | 1:500:A:PRO:O    | 1:504:A:GLN:H    | 18       | 0.31          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG21 | 3        | 0.3           |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG22 | 3        | 0.3           |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG23 | 3        | 0.3           |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD11 | 14       | 0.3           |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD12 | 14       | 0.3           |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD13 | 14       | 0.3           |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 2        | 0.3           |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 2        | 0.3           |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 10       | 0.3           |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 10       | 0.3           |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 18       | 0.3           |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 18       | 0.3           |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 18       | 0.3           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 8        | 0.3           |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 8        | 0.3           |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 8        | 0.3           |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE1  | 5        | 0.3           |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE2  | 5        | 0.3           |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 17       | 0.3           |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 17       | 0.3           |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 12       | 0.3           |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 20       | 0.3           |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 20       | 0.3           |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 20       | 0.3           |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 20       | 0.3           |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 1        | 0.3           |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 1        | 0.3           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 13       | 0.3           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 13       | 0.3           |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 13       | 0.3           |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 13       | 0.3           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 13       | 0.3           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 13       | 0.3           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 13       | 0.3           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 13       | 0.3           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 13       | 0.3           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 13       | 0.3           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 13       | 0.3           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 13       | 0.3           |
| (3,270) | 1:459:A:ILE:HD11 | 1:493:A:CYS:HB2  | 5        | 0.3           |
| (3,270) | 1:459:A:ILE:HD12 | 1:493:A:CYS:HB2  | 5        | 0.3           |
| (3,270) | 1:459:A:ILE:HD13 | 1:493:A:CYS:HB2  | 5        | 0.3           |
| (3,270) | 1:459:A:ILE:HD11 | 1:493:A:CYS:HB3  | 5        | 0.3           |
| (3,270) | 1:459:A:ILE:HD12 | 1:493:A:CYS:HB3  | 5        | 0.3           |
| (3,270) | 1:459:A:ILE:HD13 | 1:493:A:CYS:HB3  | 5        | 0.3           |
| (3,260) | 1:490:A:ASP:HB3  | 1:492:A:GLU:HG2  | 9        | 0.3           |
| (3,260) | 1:490:A:ASP:HB3  | 1:492:A:GLU:HG3  | 9        | 0.3           |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 9        | 0.3           |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 9        | 0.3           |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 9        | 0.3           |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 9        | 0.3           |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 9        | 0.3           |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 9        | 0.3           |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD11 | 16       | 0.3           |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD12 | 16       | 0.3           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD13 | 16       | 0.3           |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD21 | 16       | 0.3           |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD22 | 16       | 0.3           |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD23 | 16       | 0.3           |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 4        | 0.3           |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 4        | 0.3           |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 4        | 0.3           |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 4        | 0.3           |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 4        | 0.3           |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 4        | 0.3           |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG2  | 8        | 0.29          |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG3  | 8        | 0.29          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD11 | 14       | 0.29          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD12 | 14       | 0.29          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD13 | 14       | 0.29          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD11 | 5        | 0.29          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD12 | 5        | 0.29          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD13 | 5        | 0.29          |
| (3,731) | 1:451:A:PHE:HD1  | 1:533:A:TRP:HB3  | 17       | 0.29          |
| (3,731) | 1:451:A:PHE:HD2  | 1:533:A:TRP:HB3  | 17       | 0.29          |
| (3,725) | 1:531:A:ARG:HD2  | 1:532:A:TYR:H    | 2        | 0.29          |
| (3,725) | 1:531:A:ARG:HD3  | 1:532:A:TYR:H    | 2        | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 19       | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 19       | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 19       | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 19       | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 19       | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 19       | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD11 | 19       | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD12 | 19       | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD13 | 19       | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD21 | 19       | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD22 | 19       | 0.29          |
| (3,620) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HD23 | 19       | 0.29          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 3        | 0.29          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 3        | 0.29          |
| (3,602) | 1:519:A:TRP:HD1  | 1:520:A:LYS:H    | 16       | 0.29          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 6        | 0.29          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 15       | 0.29          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 3        | 0.29          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 3        | 0.29          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 3        | 0.29          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,496) | 1:513:A:ILE:H    | 1:513:A:ILE:HD11 | 10       | 0.29          |
| (3,496) | 1:513:A:ILE:H    | 1:513:A:ILE:HD12 | 10       | 0.29          |
| (3,496) | 1:513:A:ILE:H    | 1:513:A:ILE:HD13 | 10       | 0.29          |
| (3,410) | 1:501:A:GLU:HG2  | 1:502:A:ASP:H    | 15       | 0.29          |
| (3,410) | 1:501:A:GLU:HG3  | 1:502:A:ASP:H    | 15       | 0.29          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 6        | 0.29          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 6        | 0.29          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 6        | 0.29          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 6        | 0.29          |
| (3,350) | 1:496:A:ARG:H    | 1:496:A:ARG:HD2  | 20       | 0.29          |
| (3,350) | 1:496:A:ARG:H    | 1:496:A:ARG:HD3  | 20       | 0.29          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB1  | 11       | 0.29          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB2  | 11       | 0.29          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB3  | 11       | 0.29          |
| (3,303) | 1:459:A:ILE:HG12 | 1:494:A:HIS:HA   | 10       | 0.29          |
| (3,303) | 1:459:A:ILE:HG13 | 1:494:A:HIS:HA   | 10       | 0.29          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 2        | 0.29          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 2        | 0.29          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 11       | 0.29          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 11       | 0.29          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 8        | 0.29          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 14       | 0.29          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 14       | 0.29          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 14       | 0.29          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 14       | 0.29          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 14       | 0.29          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 14       | 0.29          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 14       | 0.29          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 14       | 0.29          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 14       | 0.29          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 14       | 0.29          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 14       | 0.29          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 14       | 0.29          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 4        | 0.29          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 4        | 0.29          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 4        | 0.29          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 4        | 0.29          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 6        | 0.29          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 6        | 0.29          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG21 | 20       | 0.29          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG22 | 20       | 0.29          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG23 | 20       | 0.29          |
| (3,913) | 1:558:A:ILE:HG21 | 1:559:A:THR:H    | 12       | 0.28          |
| (3,913) | 1:558:A:ILE:HG22 | 1:559:A:THR:H    | 12       | 0.28          |
| (3,913) | 1:558:A:ILE:HG23 | 1:559:A:THR:H    | 12       | 0.28          |
| (3,896) | 1:553:A:GLY:H    | 1:554:A:THR:H    | 3        | 0.28          |
| (3,890) | 1:550:A:LYS:H    | 1:550:A:LYS:HG2  | 18       | 0.28          |
| (3,890) | 1:550:A:LYS:H    | 1:550:A:LYS:HG3  | 18       | 0.28          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG2  | 18       | 0.28          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG3  | 18       | 0.28          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG2  | 18       | 0.28          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG3  | 18       | 0.28          |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2  | 12       | 0.28          |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2  | 12       | 0.28          |
| (3,725) | 1:531:A:ARG:HD2  | 1:532:A:TYR:H    | 18       | 0.28          |
| (3,725) | 1:531:A:ARG:HD3  | 1:532:A:TYR:H    | 18       | 0.28          |
| (3,720) | 1:524:A:LEU:HD11 | 1:532:A:TYR:HD2  | 18       | 0.28          |
| (3,720) | 1:524:A:LEU:HD12 | 1:532:A:TYR:HD2  | 18       | 0.28          |
| (3,720) | 1:524:A:LEU:HD13 | 1:532:A:TYR:HD2  | 18       | 0.28          |
| (3,720) | 1:524:A:LEU:HD21 | 1:532:A:TYR:HD2  | 18       | 0.28          |
| (3,720) | 1:524:A:LEU:HD22 | 1:532:A:TYR:HD2  | 18       | 0.28          |
| (3,720) | 1:524:A:LEU:HD23 | 1:532:A:TYR:HD2  | 18       | 0.28          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 15       | 0.28          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 15       | 0.28          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 2        | 0.28          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 2        | 0.28          |
| (3,653) | 1:524:A:LEU:H    | 1:524:A:LEU:HG   | 17       | 0.28          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD11 | 9        | 0.28          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD12 | 9        | 0.28          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD13 | 9        | 0.28          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD21 | 9        | 0.28          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD22 | 9        | 0.28          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD23 | 9        | 0.28          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 2        | 0.28          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 2        | 0.28          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 2        | 0.28          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 2        | 0.28          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 2        | 0.28          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 2        | 0.28          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 12       | 0.28          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 12       | 0.28          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 1        | 0.28          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 1        | 0.28          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 13       | 0.28          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 14       | 0.28          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 18       | 0.28          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 19       | 0.28          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 4        | 0.28          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 1        | 0.28          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 1        | 0.28          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 1        | 0.28          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 16       | 0.28          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 16       | 0.28          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 16       | 0.28          |
| (3,410) | 1:501:A:GLU:HG2  | 1:502:A:ASP:H    | 3        | 0.28          |
| (3,410) | 1:501:A:GLU:HG3  | 1:502:A:ASP:H    | 3        | 0.28          |
| (3,410) | 1:501:A:GLU:HG2  | 1:502:A:ASP:H    | 13       | 0.28          |
| (3,410) | 1:501:A:GLU:HG3  | 1:502:A:ASP:H    | 13       | 0.28          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 12       | 0.28          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 12       | 0.28          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 8        | 0.28          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 8        | 0.28          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 12       | 0.28          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 12       | 0.28          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 8        | 0.28          |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG2  | 8        | 0.28          |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG3  | 8        | 0.28          |
| (3,233) | 1:486:A:LEU:HG   | 1:487:A:LEU:H    | 3        | 0.28          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB2  | 10       | 0.28          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB3  | 10       | 0.28          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB2  | 10       | 0.28          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB3  | 10       | 0.28          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB2  | 16       | 0.28          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB3  | 16       | 0.28          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB2  | 16       | 0.28          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB3  | 16       | 0.28          |
| (3,93)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HG   | 12       | 0.28          |
| (3,93)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HG   | 12       | 0.28          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 12       | 0.28          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 12       | 0.28          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 12       | 0.28          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 12       | 0.28          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 12       | 0.28          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 12       | 0.28          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 8        | 0.28          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 8        | 0.28          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 8        | 0.28          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 8        | 0.28          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 8        | 0.28          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 8        | 0.28          |
| (3,29)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HA   | 6        | 0.28          |
| (3,29)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HA   | 6        | 0.28          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 12       | 0.28          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 12       | 0.28          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 12       | 0.28          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 12       | 0.28          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 12       | 0.28          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 12       | 0.28          |
| (1,35)  | 1:500:A:PRO:O    | 1:504:A:GLN:H    | 12       | 0.28          |
| (3,874) | 1:545:A:ASN:H    | 1:546:A:GLN:H    | 19       | 0.27          |
| (3,695) | 1:451:A:PHE:HE1  | 1:530:A:GLN:HA   | 8        | 0.27          |
| (3,695) | 1:451:A:PHE:HE2  | 1:530:A:GLN:HA   | 8        | 0.27          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD11 | 13       | 0.27          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD12 | 13       | 0.27          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD13 | 13       | 0.27          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD21 | 13       | 0.27          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD22 | 13       | 0.27          |
| (3,649) | 1:494:A:HIS:HD2  | 1:524:A:LEU:HD23 | 13       | 0.27          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 14       | 0.27          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 14       | 0.27          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 14       | 0.27          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 14       | 0.27          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 14       | 0.27          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 14       | 0.27          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 15       | 0.27          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 15       | 0.27          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 10       | 0.27          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 18       | 0.27          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 18       | 0.27          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 13       | 0.27          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 13       | 0.27          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 1        | 0.27          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 14       | 0.27          |
| (3,325) | 1:485:A:ASP:H    | 1:495:A:ALA:HA   | 6        | 0.27          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 14       | 0.27          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 14       | 0.27          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 3        | 0.27          |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG2  | 11       | 0.27          |
| (3,238) | 1:488:A:GLU:H    | 1:488:A:GLU:HG3  | 11       | 0.27          |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD2  | 15       | 0.27          |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD3  | 15       | 0.27          |
| (3,6)   | 1:446:A:ALA:HB1  | 1:447:A:THR:H    | 13       | 0.27          |
| (3,6)   | 1:446:A:ALA:HB2  | 1:447:A:THR:H    | 13       | 0.27          |
| (3,6)   | 1:446:A:ALA:HB3  | 1:447:A:THR:H    | 13       | 0.27          |
| (1,45)  | 1:505:A:ALA:O    | 1:509:A:ALA:H    | 7        | 0.27          |
| (1,38)  | 1:501:A:GLU:O    | 1:505:A:ALA:N    | 5        | 0.27          |
| (3,911) | 1:558:A:ILE:HB   | 1:559:A:THR:H    | 2        | 0.26          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG21 | 15       | 0.26          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG22 | 15       | 0.26          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG23 | 15       | 0.26          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 8        | 0.26          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 8        | 0.26          |
| (3,746) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HZ2  | 3        | 0.26          |
| (3,746) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HZ2  | 3        | 0.26          |
| (3,725) | 1:531:A:ARG:HD2  | 1:532:A:TYR:H    | 1        | 0.26          |
| (3,725) | 1:531:A:ARG:HD3  | 1:532:A:TYR:H    | 1        | 0.26          |
| (3,706) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 1        | 0.26          |
| (3,706) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 1        | 0.26          |
| (3,706) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 5        | 0.26          |
| (3,706) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 5        | 0.26          |
| (3,699) | 1:529:A:GLU:HG2  | 1:530:A:GLN:HA   | 19       | 0.26          |
| (3,699) | 1:529:A:GLU:HG3  | 1:530:A:GLN:HA   | 19       | 0.26          |
| (3,689) | 1:526:A:GLY:H    | 1:529:A:GLU:HG2  | 7        | 0.26          |
| (3,689) | 1:526:A:GLY:H    | 1:529:A:GLU:HG3  | 7        | 0.26          |
| (3,619) | 1:510:A:TYR:HB3  | 1:521:A:LEU:HG   | 20       | 0.26          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB2  | 18       | 0.26          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB3  | 18       | 0.26          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 8        | 0.26          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 15       | 0.26          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 15       | 0.26          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 15       | 0.26          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 12       | 0.26          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 12       | 0.26          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 12       | 0.26          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 17       | 0.26          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 17       | 0.26          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 17       | 0.26          |
| (3,457) | 1:507:A:ILE:HD11 | 1:508:A:ASN:HD22 | 1        | 0.26          |
| (3,457) | 1:507:A:ILE:HD12 | 1:508:A:ASN:HD22 | 1        | 0.26          |
| (3,457) | 1:507:A:ILE:HD13 | 1:508:A:ASN:HD22 | 1        | 0.26          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 1        | 0.26          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 1        | 0.26          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 1        | 0.26          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 1        | 0.26          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 12       | 0.26          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 12       | 0.26          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 1        | 0.26          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 1        | 0.26          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 2        | 0.26          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD2  | 12       | 0.26          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD2  | 12       | 0.26          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD2  | 12       | 0.26          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD3  | 12       | 0.26          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD3  | 12       | 0.26          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD3  | 12       | 0.26          |
| (3,303) | 1:459:A:ILE:HG12 | 1:494:A:HIS:HA   | 13       | 0.26          |
| (3,303) | 1:459:A:ILE:HG13 | 1:494:A:HIS:HA   | 13       | 0.26          |
| (3,303) | 1:459:A:ILE:HG12 | 1:494:A:HIS:HA   | 18       | 0.26          |
| (3,303) | 1:459:A:ILE:HG13 | 1:494:A:HIS:HA   | 18       | 0.26          |
| (3,298) | 1:458:A:LYS:HD2  | 1:494:A:HIS:HE1  | 2        | 0.26          |
| (3,298) | 1:458:A:LYS:HD3  | 1:494:A:HIS:HE1  | 2        | 0.26          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 7        | 0.26          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 7        | 0.26          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 10       | 0.26          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 10       | 0.26          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 2        | 0.26          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 2        | 0.26          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 2        | 0.26          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 2        | 0.26          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 2        | 0.26          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 2        | 0.26          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 2        | 0.26          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 2        | 0.26          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 2        | 0.26          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 2        | 0.26          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 2        | 0.26          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 2        | 0.26          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 15       | 0.26          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 16       | 0.26          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 16       | 0.26          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 16       | 0.26          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 16       | 0.26          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 16       | 0.26          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 16       | 0.26          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB2  | 15       | 0.26          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB2  | 15       | 0.26          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB3  | 15       | 0.26          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB3  | 15       | 0.26          |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD2  | 8        | 0.25          |
| (3,881) | 1:548:A:ARG:H    | 1:548:A:ARG:HD3  | 8        | 0.25          |
| (3,879) | 1:547:A:PRO:HB2  | 1:548:A:ARG:H    | 1        | 0.25          |
| (3,879) | 1:547:A:PRO:HB3  | 1:548:A:ARG:H    | 1        | 0.25          |
| (3,879) | 1:547:A:PRO:HB2  | 1:548:A:ARG:H    | 13       | 0.25          |
| (3,879) | 1:547:A:PRO:HB3  | 1:548:A:ARG:H    | 13       | 0.25          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD11 | 3        | 0.25          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD12 | 3        | 0.25          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD13 | 3        | 0.25          |
| (3,779) | 1:534:A:GLN:HA   | 1:534:A:GLN:HE21 | 17       | 0.25          |
| (3,779) | 1:534:A:GLN:HA   | 1:534:A:GLN:HE22 | 17       | 0.25          |
| (3,730) | 1:451:A:PHE:HZ   | 1:533:A:TRP:HD1  | 8        | 0.25          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 14       | 0.25          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 14       | 0.25          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 17       | 0.25          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 17       | 0.25          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 17       | 0.25          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 17       | 0.25          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 17       | 0.25          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 17       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 1        | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 10       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 10       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 10       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 10       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 10       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 10       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 10       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 10       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 10       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 10       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 10       | 0.25          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 10       | 0.25          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 5        | 0.25          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 9        | 0.25          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 10       | 0.25          |
| (3,515) | 1:515:A:LYS:H    | 1:515:A:LYS:HG2  | 13       | 0.25          |
| (3,515) | 1:515:A:LYS:H    | 1:515:A:LYS:HG3  | 13       | 0.25          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 9        | 0.25          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 9        | 0.25          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 9        | 0.25          |
| (3,410) | 1:501:A:GLU:HG2  | 1:502:A:ASP:H    | 16       | 0.25          |
| (3,410) | 1:501:A:GLU:HG3  | 1:502:A:ASP:H    | 16       | 0.25          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB2  | 9        | 0.25          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB3  | 9        | 0.25          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB2  | 9        | 0.25          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB3  | 9        | 0.25          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 11       | 0.25          |
| (3,297) | 1:458:A:LYS:HD2  | 1:494:A:HIS:HD2  | 12       | 0.25          |
| (3,297) | 1:458:A:LYS:HD3  | 1:494:A:HIS:HD2  | 12       | 0.25          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 20       | 0.25          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 20       | 0.25          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 20       | 0.25          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 20       | 0.25          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 11       | 0.25          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB2  | 12       | 0.25          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB2  | 12       | 0.25          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB2  | 12       | 0.25          |
| (3,273) | 1:465:A:LEU:HD11 | 1:493:A:CYS:HB3  | 12       | 0.25          |
| (3,273) | 1:465:A:LEU:HD12 | 1:493:A:CYS:HB3  | 12       | 0.25          |
| (3,273) | 1:465:A:LEU:HD13 | 1:493:A:CYS:HB3  | 12       | 0.25          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB2  | 12       | 0.25          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB2  | 12       | 0.25          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB2  | 12       | 0.25          |
| (3,273) | 1:465:A:LEU:HD21 | 1:493:A:CYS:HB3  | 12       | 0.25          |
| (3,273) | 1:465:A:LEU:HD22 | 1:493:A:CYS:HB3  | 12       | 0.25          |
| (3,273) | 1:465:A:LEU:HD23 | 1:493:A:CYS:HB3  | 12       | 0.25          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 20       | 0.25          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 20       | 0.25          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 20       | 0.25          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 20       | 0.25          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 20       | 0.25          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 20       | 0.25          |
| (3,233) | 1:486:A:LEU:HG   | 1:487:A:LEU:H    | 6        | 0.25          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD11 | 2        | 0.25          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD12 | 2        | 0.25          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD13 | 2        | 0.25          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD21 | 2        | 0.25          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD22 | 2        | 0.25          |
| (3,231) | 1:486:A:LEU:HA   | 1:486:A:LEU:HD23 | 2        | 0.25          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD11 | 6        | 0.25          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD12 | 6        | 0.25          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD13 | 6        | 0.25          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD21 | 6        | 0.25          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD22 | 6        | 0.25          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD23 | 6        | 0.25          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 19       | 0.25          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 19       | 0.25          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 19       | 0.25          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 19       | 0.25          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 19       | 0.25          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 19       | 0.25          |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD2  | 20       | 0.25          |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD3  | 20       | 0.25          |
| (3,1)   | 1:445:A:ASN:HB2  | 1:446:A:ALA:H    | 6        | 0.25          |
| (1,43)  | 1:504:A:GLN:O    | 1:508:A:ASN:H    | 17       | 0.25          |
| (3,913) | 1:558:A:ILE:HG21 | 1:559:A:THR:H    | 13       | 0.24          |
| (3,913) | 1:558:A:ILE:HG22 | 1:559:A:THR:H    | 13       | 0.24          |
| (3,913) | 1:558:A:ILE:HG23 | 1:559:A:THR:H    | 13       | 0.24          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD11 | 9        | 0.24          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD12 | 9        | 0.24          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD13 | 9        | 0.24          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 13       | 0.24          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 13       | 0.24          |
| (3,695) | 1:451:A:PHE:HE1  | 1:530:A:GLN:HA   | 5        | 0.24          |
| (3,695) | 1:451:A:PHE:HE2  | 1:530:A:GLN:HA   | 5        | 0.24          |
| (3,689) | 1:526:A:GLY:H    | 1:529:A:GLU:HG2  | 18       | 0.24          |
| (3,689) | 1:526:A:GLY:H    | 1:529:A:GLU:HG3  | 18       | 0.24          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB2  | 18       | 0.24          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB3  | 18       | 0.24          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 5        | 0.24          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 7        | 0.24          |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD21 | 3        | 0.24          |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD21 | 3        | 0.24          |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD22 | 3        | 0.24          |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD22 | 3        | 0.24          |
| (3,412) | 1:455:A:VAL:HG11 | 1:503:A:ALA:H    | 13       | 0.24          |
| (3,412) | 1:455:A:VAL:HG12 | 1:503:A:ALA:H    | 13       | 0.24          |
| (3,412) | 1:455:A:VAL:HG13 | 1:503:A:ALA:H    | 13       | 0.24          |
| (3,412) | 1:455:A:VAL:HG21 | 1:503:A:ALA:H    | 13       | 0.24          |
| (3,412) | 1:455:A:VAL:HG22 | 1:503:A:ALA:H    | 13       | 0.24          |
| (3,412) | 1:455:A:VAL:HG23 | 1:503:A:ALA:H    | 13       | 0.24          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 3        | 0.24          |
| (3,325) | 1:485:A:ASP:H    | 1:495:A:ALA:HA   | 3        | 0.24          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 1        | 0.24          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 1        | 0.24          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 1        | 0.24          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 1        | 0.24          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 20       | 0.24          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 20       | 0.24          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 3        | 0.24          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 13       | 0.24          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 13       | 0.24          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 13       | 0.24          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 13       | 0.24          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 13       | 0.24          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 13       | 0.24          |
| (1,39)  | 1:502:A:ASP:O    | 1:506:A:VAL:H    | 6        | 0.24          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG21 | 8        | 0.23          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG22 | 8        | 0.23          |
| (3,914) | 1:559:A:THR:H    | 1:559:A:THR:HG23 | 8        | 0.23          |
| (3,911) | 1:558:A:ILE:HB   | 1:559:A:THR:H    | 13       | 0.23          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG2  | 16       | 0.23          |
| (3,892) | 1:551:A:LYS:H    | 1:551:A:LYS:HG3  | 16       | 0.23          |
| (3,849) | 1:537:A:LEU:HB2  | 1:538:A:VAL:H    | 4        | 0.23          |
| (3,849) | 1:537:A:LEU:HB3  | 1:538:A:VAL:H    | 4        | 0.23          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD11 | 7        | 0.23          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD12 | 7        | 0.23          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD13 | 7        | 0.23          |
| (3,755) | 1:529:A:GLU:HG2  | 1:533:A:TRP:HD1  | 16       | 0.23          |
| (3,755) | 1:529:A:GLU:HG3  | 1:533:A:TRP:HD1  | 16       | 0.23          |
| (3,694) | 1:451:A:PHE:HZ   | 1:530:A:GLN:HA   | 3        | 0.23          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 10       | 0.23          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 10       | 0.23          |
| (3,561) | 1:461:A:SER:HB2  | 1:519:A:TRP:HD1  | 10       | 0.23          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 11       | 0.23          |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD21 | 11       | 0.23          |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD21 | 11       | 0.23          |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD22 | 11       | 0.23          |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD22 | 11       | 0.23          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,457) | 1:507:A:ILE:HD11 | 1:508:A:ASN:HD22 | 3        | 0.23          |
| (3,457) | 1:507:A:ILE:HD12 | 1:508:A:ASN:HD22 | 3        | 0.23          |
| (3,457) | 1:507:A:ILE:HD13 | 1:508:A:ASN:HD22 | 3        | 0.23          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 2        | 0.23          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 2        | 0.23          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD2  | 10       | 0.23          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD2  | 10       | 0.23          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD2  | 10       | 0.23          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD3  | 10       | 0.23          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD3  | 10       | 0.23          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD3  | 10       | 0.23          |
| (3,333) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HA   | 7        | 0.23          |
| (3,333) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HA   | 7        | 0.23          |
| (3,333) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HA   | 7        | 0.23          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB2  | 13       | 0.23          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB3  | 13       | 0.23          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB2  | 13       | 0.23          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB3  | 13       | 0.23          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 9        | 0.23          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 9        | 0.23          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 9        | 0.23          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 9        | 0.23          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 9        | 0.23          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 9        | 0.23          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 7        | 0.23          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 7        | 0.23          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 18       | 0.23          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 18       | 0.23          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 18       | 0.23          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 18       | 0.23          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 18       | 0.23          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 18       | 0.23          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 3        | 0.23          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 3        | 0.23          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 3        | 0.23          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 3        | 0.23          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 3        | 0.23          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 3        | 0.23          |
| (3,6)   | 1:446:A:ALA:HB1  | 1:447:A:THR:H    | 18       | 0.23          |
| (3,6)   | 1:446:A:ALA:HB2  | 1:447:A:THR:H    | 18       | 0.23          |
| (3,6)   | 1:446:A:ALA:HB3  | 1:447:A:THR:H    | 18       | 0.23          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD11 | 18       | 0.22          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD12 | 18       | 0.22          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD13 | 18       | 0.22          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD2  | 4        | 0.22          |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD3  | 4        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 7        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 7        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 7        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 7        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 7        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 7        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 7        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 7        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 7        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 7        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 7        | 0.22          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 7        | 0.22          |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD2  | 15       | 0.22          |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD3  | 15       | 0.22          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 8        | 0.22          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 8        | 0.22          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 8        | 0.22          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 8        | 0.22          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 8        | 0.22          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 8        | 0.22          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 20       | 0.22          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 20       | 0.22          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 20       | 0.22          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 20       | 0.22          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 20       | 0.22          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 20       | 0.22          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 1        | 0.22          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE2  | 18       | 0.22          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE3  | 18       | 0.22          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE2  | 18       | 0.22          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE3  | 18       | 0.22          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE2  | 19       | 0.22          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE3  | 19       | 0.22          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE2  | 19       | 0.22          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE3  | 19       | 0.22          |
| (3,457) | 1:507:A:ILE:HD11 | 1:508:A:ASN:HD22 | 19       | 0.22          |
| (3,457) | 1:507:A:ILE:HD12 | 1:508:A:ASN:HD22 | 19       | 0.22          |
| (3,457) | 1:507:A:ILE:HD13 | 1:508:A:ASN:HD22 | 19       | 0.22          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,447) | 1:504:A:GLN:HG2  | 1:508:A:ASN:HD21 | 1        | 0.22          |
| (3,447) | 1:504:A:GLN:HG3  | 1:508:A:ASN:HD21 | 1        | 0.22          |
| (3,447) | 1:504:A:GLN:HG2  | 1:508:A:ASN:HD22 | 1        | 0.22          |
| (3,447) | 1:504:A:GLN:HG3  | 1:508:A:ASN:HD22 | 1        | 0.22          |
| (3,303) | 1:459:A:ILE:HG12 | 1:494:A:HIS:HA   | 1        | 0.22          |
| (3,303) | 1:459:A:ILE:HG13 | 1:494:A:HIS:HA   | 1        | 0.22          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 12       | 0.22          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 12       | 0.22          |
| (3,92)  | 1:461:A:SER:H    | 1:465:A:LEU:HD11 | 15       | 0.22          |
| (3,92)  | 1:461:A:SER:H    | 1:465:A:LEU:HD12 | 15       | 0.22          |
| (3,92)  | 1:461:A:SER:H    | 1:465:A:LEU:HD13 | 15       | 0.22          |
| (3,92)  | 1:461:A:SER:H    | 1:465:A:LEU:HD21 | 15       | 0.22          |
| (3,92)  | 1:461:A:SER:H    | 1:465:A:LEU:HD22 | 15       | 0.22          |
| (3,92)  | 1:461:A:SER:H    | 1:465:A:LEU:HD23 | 15       | 0.22          |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD2  | 11       | 0.22          |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD3  | 11       | 0.22          |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD2  | 14       | 0.22          |
| (3,86)  | 1:462:A:THR:H    | 1:464:A:PRO:HD3  | 14       | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 4        | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 4        | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 4        | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 4        | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 4        | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 4        | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 17       | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 17       | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 17       | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 17       | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 17       | 0.22          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 17       | 0.22          |
| (1,38)  | 1:501:A:GLU:O    | 1:505:A:ALA:N    | 18       | 0.22          |
| (3,879) | 1:547:A:PRO:HB2  | 1:548:A:ARG:H    | 15       | 0.21          |
| (3,879) | 1:547:A:PRO:HB3  | 1:548:A:ARG:H    | 15       | 0.21          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD21 | 11       | 0.21          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD22 | 11       | 0.21          |
| (3,858) | 1:536:A:ILE:HG21 | 1:540:A:ARG:HD2  | 18       | 0.21          |
| (3,858) | 1:536:A:ILE:HG21 | 1:540:A:ARG:HD3  | 18       | 0.21          |
| (3,858) | 1:536:A:ILE:HG22 | 1:540:A:ARG:HD2  | 18       | 0.21          |
| (3,858) | 1:536:A:ILE:HG22 | 1:540:A:ARG:HD3  | 18       | 0.21          |
| (3,858) | 1:536:A:ILE:HG23 | 1:540:A:ARG:HD2  | 18       | 0.21          |
| (3,858) | 1:536:A:ILE:HG23 | 1:540:A:ARG:HD3  | 18       | 0.21          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 18       | 0.21          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 18       | 0.21          |
| (3,775) | 1:531:A:ARG:HA   | 1:534:A:GLN:HG2  | 17       | 0.21          |
| (3,775) | 1:531:A:ARG:HA   | 1:534:A:GLN:HG3  | 17       | 0.21          |
| (3,725) | 1:531:A:ARG:HD2  | 1:532:A:TYR:H    | 7        | 0.21          |
| (3,725) | 1:531:A:ARG:HD3  | 1:532:A:TYR:H    | 7        | 0.21          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 18       | 0.21          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 18       | 0.21          |
| (3,694) | 1:451:A:PHE:HZ   | 1:530:A:GLN:HA   | 11       | 0.21          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB2  | 5        | 0.21          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB3  | 5        | 0.21          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB2  | 12       | 0.21          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB3  | 12       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 11       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 11       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 11       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 11       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 11       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 11       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 11       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 11       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 11       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 11       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 11       | 0.21          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 11       | 0.21          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 6        | 0.21          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 6        | 0.21          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 6        | 0.21          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE1  | 7        | 0.21          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE2  | 7        | 0.21          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE1  | 15       | 0.21          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE2  | 15       | 0.21          |
| (3,412) | 1:455:A:VAL:HG11 | 1:503:A:ALA:H    | 4        | 0.21          |
| (3,412) | 1:455:A:VAL:HG12 | 1:503:A:ALA:H    | 4        | 0.21          |
| (3,412) | 1:455:A:VAL:HG13 | 1:503:A:ALA:H    | 4        | 0.21          |
| (3,412) | 1:455:A:VAL:HG21 | 1:503:A:ALA:H    | 4        | 0.21          |
| (3,412) | 1:455:A:VAL:HG22 | 1:503:A:ALA:H    | 4        | 0.21          |
| (3,412) | 1:455:A:VAL:HG23 | 1:503:A:ALA:H    | 4        | 0.21          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 6        | 0.21          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 6        | 0.21          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 20       | 0.21          |
| (3,325) | 1:485:A:ASP:H    | 1:495:A:ALA:HA   | 4        | 0.21          |
| (3,325) | 1:485:A:ASP:H    | 1:495:A:ALA:HA   | 13       | 0.21          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,325) | 1:485:A:ASP:H    | 1:495:A:ALA:HA   | 15       | 0.21          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB1  | 17       | 0.21          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB2  | 17       | 0.21          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB3  | 17       | 0.21          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB2  | 5        | 0.21          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB3  | 5        | 0.21          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB2  | 5        | 0.21          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB3  | 5        | 0.21          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB2  | 17       | 0.21          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB3  | 17       | 0.21          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB2  | 17       | 0.21          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB3  | 17       | 0.21          |
| (3,101) | 1:465:A:LEU:HD11 | 1:467:A:GLY:H    | 8        | 0.21          |
| (3,101) | 1:465:A:LEU:HD12 | 1:467:A:GLY:H    | 8        | 0.21          |
| (3,101) | 1:465:A:LEU:HD13 | 1:467:A:GLY:H    | 8        | 0.21          |
| (3,101) | 1:465:A:LEU:HD21 | 1:467:A:GLY:H    | 8        | 0.21          |
| (3,101) | 1:465:A:LEU:HD22 | 1:467:A:GLY:H    | 8        | 0.21          |
| (3,101) | 1:465:A:LEU:HD23 | 1:467:A:GLY:H    | 8        | 0.21          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 1        | 0.21          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 1        | 0.21          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 1        | 0.21          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 1        | 0.21          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 1        | 0.21          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 1        | 0.21          |
| (1,38)  | 1:501:A:GLU:O    | 1:505:A:ALA:N    | 14       | 0.21          |
| (1,37)  | 1:501:A:GLU:O    | 1:505:A:ALA:H    | 12       | 0.21          |
| (1,35)  | 1:500:A:PRO:O    | 1:504:A:GLN:H    | 11       | 0.21          |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG2  | 18       | 0.2           |
| (3,886) | 1:549:A:GLU:H    | 1:549:A:GLU:HG3  | 18       | 0.2           |
| (3,884) | 1:548:A:ARG:HD2  | 1:549:A:GLU:H    | 20       | 0.2           |
| (3,884) | 1:548:A:ARG:HD3  | 1:549:A:GLU:H    | 20       | 0.2           |
| (3,863) | 1:541:A:GLN:HA   | 1:541:A:GLN:HE21 | 12       | 0.2           |
| (3,863) | 1:541:A:GLN:HA   | 1:541:A:GLN:HE22 | 12       | 0.2           |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD2  | 6        | 0.2           |
| (3,781) | 1:532:A:TYR:HA   | 1:535:A:LYS:HD3  | 6        | 0.2           |
| (3,653) | 1:524:A:LEU:H    | 1:524:A:LEU:HG   | 13       | 0.2           |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 13       | 0.2           |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 13       | 0.2           |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 13       | 0.2           |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 13       | 0.2           |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 13       | 0.2           |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 13       | 0.2           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 13       | 0.2           |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 13       | 0.2           |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 13       | 0.2           |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 13       | 0.2           |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 13       | 0.2           |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 13       | 0.2           |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 18       | 0.2           |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 19       | 0.2           |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE2  | 14       | 0.2           |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE3  | 14       | 0.2           |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 18       | 0.2           |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 18       | 0.2           |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 18       | 0.2           |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD21 | 17       | 0.2           |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD21 | 17       | 0.2           |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD22 | 17       | 0.2           |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD22 | 17       | 0.2           |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 4        | 0.2           |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 4        | 0.2           |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 4        | 0.2           |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 4        | 0.2           |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD2  | 13       | 0.2           |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD2  | 13       | 0.2           |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD2  | 13       | 0.2           |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD3  | 13       | 0.2           |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD3  | 13       | 0.2           |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD3  | 13       | 0.2           |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 8        | 0.2           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 14       | 0.2           |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 14       | 0.2           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 14       | 0.2           |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 14       | 0.2           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 14       | 0.2           |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 14       | 0.2           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 14       | 0.2           |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 14       | 0.2           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 14       | 0.2           |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 14       | 0.2           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 14       | 0.2           |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 14       | 0.2           |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 8        | 0.2           |
| (3,233) | 1:486:A:LEU:HG   | 1:487:A:LEU:H    | 4        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 3        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 3        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 3        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 3        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 3        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 3        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 9        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 9        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 9        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 9        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 9        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 9        | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 14       | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 14       | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 14       | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 14       | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 14       | 0.2           |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 14       | 0.2           |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB2  | 5        | 0.2           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB2  | 5        | 0.2           |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB3  | 5        | 0.2           |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB3  | 5        | 0.2           |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG21 | 15       | 0.2           |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG22 | 15       | 0.2           |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG23 | 15       | 0.2           |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 6        | 0.2           |
| (1,71)  | 1:531:A:ARG:O    | 1:535:A:LYS:H    | 19       | 0.2           |
| (1,43)  | 1:504:A:GLN:O    | 1:508:A:ASN:H    | 20       | 0.2           |
| (1,36)  | 1:500:A:PRO:O    | 1:504:A:GLN:N    | 5        | 0.2           |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD11 | 18       | 0.19          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD12 | 18       | 0.19          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD13 | 18       | 0.19          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD21 | 18       | 0.19          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD22 | 18       | 0.19          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD23 | 18       | 0.19          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD11 | 18       | 0.19          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD12 | 18       | 0.19          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD13 | 18       | 0.19          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD21 | 18       | 0.19          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD22 | 18       | 0.19          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD23 | 18       | 0.19          |
| (3,875) | 1:545:A:ASN:HD21 | 1:546:A:GLN:H    | 16       | 0.19          |
| (3,875) | 1:545:A:ASN:HD22 | 1:546:A:GLN:H    | 16       | 0.19          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG21 | 2        | 0.19          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG22 | 2        | 0.19          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG23 | 2        | 0.19          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG21 | 15       | 0.19          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG22 | 15       | 0.19          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG23 | 15       | 0.19          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG2  | 11       | 0.19          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG3  | 11       | 0.19          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG2  | 11       | 0.19          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG3  | 11       | 0.19          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 19       | 0.19          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 19       | 0.19          |
| (3,694) | 1:451:A:PHE:HZ   | 1:530:A:GLN:HA   | 14       | 0.19          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB2  | 7        | 0.19          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB3  | 7        | 0.19          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 6        | 0.19          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 6        | 0.19          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 6        | 0.19          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 6        | 0.19          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 6        | 0.19          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 6        | 0.19          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 6        | 0.19          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 6        | 0.19          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 6        | 0.19          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 6        | 0.19          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 6        | 0.19          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 6        | 0.19          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 16       | 0.19          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 16       | 0.19          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 16       | 0.19          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 16       | 0.19          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 16       | 0.19          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 16       | 0.19          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 19       | 0.19          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 19       | 0.19          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 19       | 0.19          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 19       | 0.19          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 19       | 0.19          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 19       | 0.19          |
| (3,561) | 1:461:A:SER:HB2  | 1:519:A:TRP:HD1  | 14       | 0.19          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 1        | 0.19          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 14       | 0.19          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE2  | 6        | 0.19          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE3  | 6        | 0.19          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE2  | 6        | 0.19          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE3  | 6        | 0.19          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE2  | 13       | 0.19          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE3  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG11 | 1:497:A:PHE:HE1  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG11 | 1:497:A:PHE:HE2  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG12 | 1:497:A:PHE:HE1  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG12 | 1:497:A:PHE:HE2  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG13 | 1:497:A:PHE:HE1  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG13 | 1:497:A:PHE:HE2  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG21 | 1:497:A:PHE:HE1  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG21 | 1:497:A:PHE:HE2  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG22 | 1:497:A:PHE:HE1  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG22 | 1:497:A:PHE:HE2  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG23 | 1:497:A:PHE:HE1  | 13       | 0.19          |
| (3,361) | 1:457:A:VAL:HG23 | 1:497:A:PHE:HE2  | 13       | 0.19          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 16       | 0.19          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 16       | 0.19          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 7        | 0.19          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 7        | 0.19          |
| (3,303) | 1:459:A:ILE:HG12 | 1:494:A:HIS:HA   | 12       | 0.19          |
| (3,303) | 1:459:A:ILE:HG13 | 1:494:A:HIS:HA   | 12       | 0.19          |
| (3,261) | 1:491:A:THR:H    | 1:492:A:GLU:HG2  | 15       | 0.19          |
| (3,261) | 1:491:A:THR:H    | 1:492:A:GLU:HG3  | 15       | 0.19          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD11 | 1        | 0.19          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD12 | 1        | 0.19          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD13 | 1        | 0.19          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD21 | 1        | 0.19          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD22 | 1        | 0.19          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD23 | 1        | 0.19          |
| (3,227) | 1:468:A:ARG:HD2  | 1:486:A:LEU:HD11 | 9        | 0.19          |
| (3,227) | 1:468:A:ARG:HD2  | 1:486:A:LEU:HD12 | 9        | 0.19          |
| (3,227) | 1:468:A:ARG:HD2  | 1:486:A:LEU:HD13 | 9        | 0.19          |
| (3,227) | 1:468:A:ARG:HD2  | 1:486:A:LEU:HD21 | 9        | 0.19          |
| (3,227) | 1:468:A:ARG:HD2  | 1:486:A:LEU:HD22 | 9        | 0.19          |
| (3,227) | 1:468:A:ARG:HD2  | 1:486:A:LEU:HD23 | 9        | 0.19          |
| (3,227) | 1:468:A:ARG:HD3  | 1:486:A:LEU:HD11 | 9        | 0.19          |
| (3,227) | 1:468:A:ARG:HD3  | 1:486:A:LEU:HD12 | 9        | 0.19          |
| (3,227) | 1:468:A:ARG:HD3  | 1:486:A:LEU:HD13 | 9        | 0.19          |
| (3,227) | 1:468:A:ARG:HD3  | 1:486:A:LEU:HD21 | 9        | 0.19          |
| (3,227) | 1:468:A:ARG:HD3  | 1:486:A:LEU:HD22 | 9        | 0.19          |
| (3,227) | 1:468:A:ARG:HD3  | 1:486:A:LEU:HD23 | 9        | 0.19          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB2  | 3        | 0.19          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB3  | 3        | 0.19          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB2  | 3        | 0.19          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB3  | 3        | 0.19          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB2  | 7        | 0.19          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB3  | 7        | 0.19          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB2  | 7        | 0.19          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB3  | 7        | 0.19          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB2  | 9        | 0.19          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB3  | 9        | 0.19          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB2  | 9        | 0.19          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB3  | 9        | 0.19          |
| (3,112) | 1:468:A:ARG:HG2  | 1:469:A:LYS:H    | 20       | 0.19          |
| (3,112) | 1:468:A:ARG:HG3  | 1:469:A:LYS:H    | 20       | 0.19          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD11 | 1        | 0.19          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD12 | 1        | 0.19          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD13 | 1        | 0.19          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD21 | 1        | 0.19          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD22 | 1        | 0.19          |
| (3,91)  | 1:460:A:ILE:HA   | 1:465:A:LEU:HD23 | 1        | 0.19          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB2  | 6        | 0.19          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB2  | 6        | 0.19          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB3  | 6        | 0.19          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB3  | 6        | 0.19          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG11 | 5        | 0.19          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG12 | 5        | 0.19          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG13 | 5        | 0.19          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG21 | 5        | 0.19          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG22 | 5        | 0.19          |
| (3,23)  | 1:452:A:VAL:H    | 1:452:A:VAL:HG23 | 5        | 0.19          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG21 | 17       | 0.19          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG22 | 17       | 0.19          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG23 | 17       | 0.19          |
| (1,43)  | 1:504:A:GLN:O    | 1:508:A:ASN:H    | 12       | 0.19          |
| (1,40)  | 1:502:A:ASP:O    | 1:506:A:VAL:N    | 18       | 0.19          |
| (3,900) | 1:554:A:THR:HG21 | 1:555:A:GLU:H    | 2        | 0.18          |
| (3,900) | 1:554:A:THR:HG22 | 1:555:A:GLU:H    | 2        | 0.18          |
| (3,900) | 1:554:A:THR:HG23 | 1:555:A:GLU:H    | 2        | 0.18          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG21 | 13       | 0.18          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG22 | 13       | 0.18          |
| (3,897) | 1:554:A:THR:H    | 1:554:A:THR:HG23 | 13       | 0.18          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD2  | 16       | 0.18          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD3  | 16       | 0.18          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD2  | 16       | 0.18          |
| (3,876) | 1:546:A:GLN:H    | 1:547:A:PRO:HD3  | 16       | 0.18          |
| (3,874) | 1:545:A:ASN:H    | 1:546:A:GLN:H    | 20       | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD11 | 7        | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD12 | 7        | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD13 | 7        | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD21 | 7        | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD22 | 7        | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD23 | 7        | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD11 | 7        | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD12 | 7        | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD13 | 7        | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD21 | 7        | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD22 | 7        | 0.18          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD23 | 7        | 0.18          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG21 | 8        | 0.18          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG22 | 8        | 0.18          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG23 | 8        | 0.18          |
| (3,825) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HB   | 19       | 0.18          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD11 | 12       | 0.18          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD12 | 12       | 0.18          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD13 | 12       | 0.18          |
| (3,748) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HZ2  | 9        | 0.18          |
| (3,748) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HZ2  | 9        | 0.18          |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2  | 10       | 0.18          |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2  | 10       | 0.18          |
| (3,733) | 1:451:A:PHE:HE1  | 1:533:A:TRP:HD1  | 5        | 0.18          |
| (3,733) | 1:451:A:PHE:HE2  | 1:533:A:TRP:HD1  | 5        | 0.18          |
| (3,706) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 10       | 0.18          |
| (3,706) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 10       | 0.18          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB2  | 16       | 0.18          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB3  | 16       | 0.18          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 7        | 0.18          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 7        | 0.18          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 7        | 0.18          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 7        | 0.18          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 7        | 0.18          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 7        | 0.18          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 19       | 0.18          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 12       | 0.18          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 15       | 0.18          |
| (3,542) | 1:514:A:ASN:HD21 | 1:518:A:CYS:H    | 10       | 0.18          |
| (3,361) | 1:457:A:VAL:HG11 | 1:497:A:PHE:HE1  | 5        | 0.18          |
| (3,361) | 1:457:A:VAL:HG11 | 1:497:A:PHE:HE2  | 5        | 0.18          |
| (3,361) | 1:457:A:VAL:HG12 | 1:497:A:PHE:HE1  | 5        | 0.18          |
| (3,361) | 1:457:A:VAL:HG12 | 1:497:A:PHE:HE2  | 5        | 0.18          |
| (3,361) | 1:457:A:VAL:HG13 | 1:497:A:PHE:HE1  | 5        | 0.18          |
| (3,361) | 1:457:A:VAL:HG13 | 1:497:A:PHE:HE2  | 5        | 0.18          |
| (3,361) | 1:457:A:VAL:HG21 | 1:497:A:PHE:HE1  | 5        | 0.18          |
| (3,361) | 1:457:A:VAL:HG21 | 1:497:A:PHE:HE2  | 5        | 0.18          |
| (3,361) | 1:457:A:VAL:HG22 | 1:497:A:PHE:HE1  | 5        | 0.18          |
| (3,361) | 1:457:A:VAL:HG22 | 1:497:A:PHE:HE2  | 5        | 0.18          |
| (3,361) | 1:457:A:VAL:HG23 | 1:497:A:PHE:HE1  | 5        | 0.18          |
| (3,361) | 1:457:A:VAL:HG23 | 1:497:A:PHE:HE2  | 5        | 0.18          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 14       | 0.18          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 14       | 0.18          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 4        | 0.18          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,325) | 1:485:A:ASP:H    | 1:495:A:ALA:HA   | 20       | 0.18          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 17       | 0.18          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 17       | 0.18          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 17       | 0.18          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 17       | 0.18          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 17       | 0.18          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 17       | 0.18          |
| (3,113) | 1:469:A:LYS:H    | 1:469:A:LYS:HG2  | 18       | 0.18          |
| (3,113) | 1:469:A:LYS:H    | 1:469:A:LYS:HG3  | 18       | 0.18          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 3        | 0.18          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 3        | 0.18          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 3        | 0.18          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 3        | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 14       | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 14       | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 14       | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 14       | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 14       | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 14       | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 20       | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 20       | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 20       | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 20       | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 20       | 0.18          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 20       | 0.18          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB2  | 4        | 0.18          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB2  | 4        | 0.18          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB3  | 4        | 0.18          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB3  | 4        | 0.18          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG21 | 1        | 0.18          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG22 | 1        | 0.18          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG23 | 1        | 0.18          |
| (1,39)  | 1:502:A:ASP:O    | 1:506:A:VAL:H    | 17       | 0.18          |
| (3,895) | 1:552:A:ARG:HB2  | 1:553:A:GLY:H    | 6        | 0.17          |
| (3,895) | 1:552:A:ARG:HB3  | 1:553:A:GLY:H    | 6        | 0.17          |
| (3,882) | 1:548:A:ARG:H    | 1:548:A:ARG:HG2  | 7        | 0.17          |
| (3,882) | 1:548:A:ARG:H    | 1:548:A:ARG:HG3  | 7        | 0.17          |
| (3,874) | 1:545:A:ASN:H    | 1:546:A:GLN:H    | 9        | 0.17          |
| (3,825) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HB   | 8        | 0.17          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 6        | 0.17          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 6        | 0.17          |
| (3,746) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HZ2  | 2        | 0.17          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,746) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HZ2  | 2        | 0.17          |
| (3,746) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HZ2  | 17       | 0.17          |
| (3,746) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HZ2  | 17       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 16       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 16       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 16       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 16       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 16       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 16       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD11 | 16       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD12 | 16       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD13 | 16       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD21 | 16       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD22 | 16       | 0.17          |
| (3,618) | 1:510:A:TYR:HB2  | 1:521:A:LEU:HD23 | 16       | 0.17          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD11 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD12 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD13 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD21 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD22 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD23 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD11 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD12 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD13 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD21 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD22 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD23 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD11 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD12 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD13 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD21 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD22 | 1        | 0.17          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD23 | 1        | 0.17          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 2        | 0.17          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 2        | 0.17          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 11       | 0.17          |
| (3,564) | 1:461:A:SER:HB2  | 1:519:A:TRP:HE1  | 9        | 0.17          |
| (3,564) | 1:461:A:SER:HB3  | 1:519:A:TRP:HE1  | 9        | 0.17          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 10       | 0.17          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 10       | 0.17          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 10       | 0.17          |
| (3,410) | 1:501:A:GLU:HG2  | 1:502:A:ASP:H    | 17       | 0.17          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,410) | 1:501:A:GLU:HG3  | 1:502:A:ASP:H    | 17       | 0.17          |
| (3,379) | 1:497:A:PHE:HB2  | 1:498:A:LYS:H    | 9        | 0.17          |
| (3,379) | 1:497:A:PHE:HB3  | 1:498:A:LYS:H    | 9        | 0.17          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE1  | 19       | 0.17          |
| (3,359) | 1:457:A:VAL:HB   | 1:497:A:PHE:HE2  | 19       | 0.17          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 1        | 0.17          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 1        | 0.17          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 15       | 0.17          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 16       | 0.17          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 17       | 0.17          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD2  | 14       | 0.17          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD2  | 14       | 0.17          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD2  | 14       | 0.17          |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD3  | 14       | 0.17          |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD3  | 14       | 0.17          |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD3  | 14       | 0.17          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB2  | 18       | 0.17          |
| (3,278) | 1:486:A:LEU:HA   | 1:493:A:CYS:HB3  | 18       | 0.17          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 2        | 0.17          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 2        | 0.17          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 2        | 0.17          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 2        | 0.17          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 2        | 0.17          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 2        | 0.17          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 2        | 0.17          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 2        | 0.17          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 2        | 0.17          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 2        | 0.17          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 2        | 0.17          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 2        | 0.17          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 11       | 0.17          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 11       | 0.17          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 11       | 0.17          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 11       | 0.17          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 11       | 0.17          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 11       | 0.17          |
| (3,183) | 1:478:A:ILE:HB   | 1:479:A:SER:HB2  | 3        | 0.17          |
| (3,183) | 1:478:A:ILE:HB   | 1:479:A:SER:HB3  | 3        | 0.17          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD11 | 4        | 0.17          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD12 | 4        | 0.17          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD13 | 4        | 0.17          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD21 | 4        | 0.17          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD22 | 4        | 0.17          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD23 | 4        | 0.17          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD11 | 13       | 0.17          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD12 | 13       | 0.17          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD13 | 13       | 0.17          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD21 | 13       | 0.17          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD22 | 13       | 0.17          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD23 | 13       | 0.17          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 13       | 0.17          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 13       | 0.17          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 13       | 0.17          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 13       | 0.17          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD2  | 3        | 0.17          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD3  | 3        | 0.17          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD2  | 10       | 0.17          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD3  | 10       | 0.17          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD2  | 13       | 0.17          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD3  | 13       | 0.17          |
| (3,34)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:HA2  | 2        | 0.17          |
| (3,34)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:HA3  | 2        | 0.17          |
| (3,34)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:HA2  | 2        | 0.17          |
| (3,34)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:HA3  | 2        | 0.17          |
| (3,34)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:HA2  | 2        | 0.17          |
| (3,34)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:HA3  | 2        | 0.17          |
| (3,34)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:HA2  | 2        | 0.17          |
| (3,34)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:HA3  | 2        | 0.17          |
| (3,34)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:HA2  | 2        | 0.17          |
| (3,34)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:HA3  | 2        | 0.17          |
| (3,34)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:HA2  | 2        | 0.17          |
| (3,34)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:HA3  | 2        | 0.17          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE21 | 15       | 0.17          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE22 | 15       | 0.17          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE21 | 16       | 0.17          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE22 | 16       | 0.17          |
| (1,43)  | 1:504:A:GLN:O    | 1:508:A:ASN:H    | 11       | 0.17          |
| (1,40)  | 1:502:A:ASP:O    | 1:506:A:VAL:N    | 5        | 0.17          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 13       | 0.16          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 13       | 0.16          |
| (3,895) | 1:552:A:ARG:HB2  | 1:553:A:GLY:H    | 2        | 0.16          |
| (3,895) | 1:552:A:ARG:HB3  | 1:553:A:GLY:H    | 2        | 0.16          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD11 | 18       | 0.16          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD12 | 18       | 0.16          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD13 | 18       | 0.16          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 7        | 0.16          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 7        | 0.16          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 10       | 0.16          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 10       | 0.16          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 14       | 0.16          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 14       | 0.16          |
| (3,775) | 1:531:A:ARG:HA   | 1:534:A:GLN:HG2  | 10       | 0.16          |
| (3,775) | 1:531:A:ARG:HA   | 1:534:A:GLN:HG3  | 10       | 0.16          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG2  | 8        | 0.16          |
| (3,773) | 1:530:A:GLN:HE21 | 1:534:A:GLN:HG3  | 8        | 0.16          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG2  | 8        | 0.16          |
| (3,773) | 1:530:A:GLN:HE22 | 1:534:A:GLN:HG3  | 8        | 0.16          |
| (3,731) | 1:451:A:PHE:HD1  | 1:533:A:TRP:HB3  | 1        | 0.16          |
| (3,731) | 1:451:A:PHE:HD2  | 1:533:A:TRP:HB3  | 1        | 0.16          |
| (3,725) | 1:531:A:ARG:HD2  | 1:532:A:TYR:H    | 20       | 0.16          |
| (3,725) | 1:531:A:ARG:HD3  | 1:532:A:TYR:H    | 20       | 0.16          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB2  | 14       | 0.16          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB3  | 14       | 0.16          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 15       | 0.16          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 15       | 0.16          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 15       | 0.16          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 15       | 0.16          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 15       | 0.16          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 15       | 0.16          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 14       | 0.16          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 20       | 0.16          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE2  | 17       | 0.16          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE3  | 17       | 0.16          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE2  | 17       | 0.16          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE3  | 17       | 0.16          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE2  | 9        | 0.16          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE3  | 9        | 0.16          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE2  | 15       | 0.16          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE3  | 15       | 0.16          |
| (3,379) | 1:497:A:PHE:HB2  | 1:498:A:LYS:H    | 4        | 0.16          |
| (3,379) | 1:497:A:PHE:HB3  | 1:498:A:LYS:H    | 4        | 0.16          |
| (3,369) | 1:481:A:VAL:HG11 | 1:497:A:PHE:HD1  | 18       | 0.16          |
| (3,369) | 1:481:A:VAL:HG11 | 1:497:A:PHE:HD2  | 18       | 0.16          |
| (3,369) | 1:481:A:VAL:HG12 | 1:497:A:PHE:HD1  | 18       | 0.16          |
| (3,369) | 1:481:A:VAL:HG12 | 1:497:A:PHE:HD2  | 18       | 0.16          |
| (3,369) | 1:481:A:VAL:HG13 | 1:497:A:PHE:HD1  | 18       | 0.16          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,369) | 1:481:A:VAL:HG13 | 1:497:A:PHE:HD2  | 18       | 0.16          |
| (3,303) | 1:459:A:ILE:HG12 | 1:494:A:HIS:HA   | 16       | 0.16          |
| (3,303) | 1:459:A:ILE:HG13 | 1:494:A:HIS:HA   | 16       | 0.16          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 10       | 0.16          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB2  | 18       | 0.16          |
| (3,276) | 1:471:A:VAL:HG11 | 1:493:A:CYS:HB3  | 18       | 0.16          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB2  | 18       | 0.16          |
| (3,276) | 1:471:A:VAL:HG12 | 1:493:A:CYS:HB3  | 18       | 0.16          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB2  | 18       | 0.16          |
| (3,276) | 1:471:A:VAL:HG13 | 1:493:A:CYS:HB3  | 18       | 0.16          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB2  | 18       | 0.16          |
| (3,276) | 1:471:A:VAL:HG21 | 1:493:A:CYS:HB3  | 18       | 0.16          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB2  | 18       | 0.16          |
| (3,276) | 1:471:A:VAL:HG22 | 1:493:A:CYS:HB3  | 18       | 0.16          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB2  | 18       | 0.16          |
| (3,276) | 1:471:A:VAL:HG23 | 1:493:A:CYS:HB3  | 18       | 0.16          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD11 | 6        | 0.16          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD12 | 6        | 0.16          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD13 | 6        | 0.16          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD21 | 6        | 0.16          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD22 | 6        | 0.16          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD23 | 6        | 0.16          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD11 | 3        | 0.16          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD12 | 3        | 0.16          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD13 | 3        | 0.16          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD21 | 3        | 0.16          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD22 | 3        | 0.16          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD23 | 3        | 0.16          |
| (3,101) | 1:465:A:LEU:HD11 | 1:467:A:GLY:H    | 4        | 0.16          |
| (3,101) | 1:465:A:LEU:HD12 | 1:467:A:GLY:H    | 4        | 0.16          |
| (3,101) | 1:465:A:LEU:HD13 | 1:467:A:GLY:H    | 4        | 0.16          |
| (3,101) | 1:465:A:LEU:HD21 | 1:467:A:GLY:H    | 4        | 0.16          |
| (3,101) | 1:465:A:LEU:HD22 | 1:467:A:GLY:H    | 4        | 0.16          |
| (3,101) | 1:465:A:LEU:HD23 | 1:467:A:GLY:H    | 4        | 0.16          |
| (3,99)  | 1:465:A:LEU:HG   | 1:467:A:GLY:H    | 9        | 0.16          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 17       | 0.16          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 17       | 0.16          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 17       | 0.16          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 17       | 0.16          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD2  | 4        | 0.16          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD3  | 4        | 0.16          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD2  | 5        | 0.16          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD3  | 5        | 0.16          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD2  | 6        | 0.16          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD3  | 6        | 0.16          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD2  | 8        | 0.16          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD3  | 8        | 0.16          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD2  | 11       | 0.16          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD3  | 11       | 0.16          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD2  | 17       | 0.16          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD3  | 17       | 0.16          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD2  | 19       | 0.16          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD3  | 19       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG11 | 12       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG12 | 12       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG13 | 12       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG21 | 12       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG22 | 12       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG23 | 12       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG11 | 15       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG12 | 15       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG13 | 15       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG21 | 15       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG22 | 15       | 0.16          |
| (3,37)  | 1:455:A:VAL:H   | 1:455:A:VAL:HG23 | 15       | 0.16          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG11 | 7        | 0.16          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG12 | 7        | 0.16          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG13 | 7        | 0.16          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG21 | 7        | 0.16          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG22 | 7        | 0.16          |
| (3,23)  | 1:452:A:VAL:H   | 1:452:A:VAL:HG23 | 7        | 0.16          |
| (3,16)  | 1:450:A:GLN:H   | 1:451:A:PHE:HD1  | 14       | 0.16          |
| (3,16)  | 1:450:A:GLN:H   | 1:451:A:PHE:HD2  | 14       | 0.16          |
| (1,43)  | 1:504:A:GLN:O   | 1:508:A:ASN:H    | 5        | 0.16          |
| (1,39)  | 1:502:A:ASP:O   | 1:506:A:VAL:H    | 14       | 0.16          |
| (3,891) | 1:550:A:LYS:HG2 | 1:551:A:LYS:H    | 10       | 0.15          |
| (3,891) | 1:550:A:LYS:HG3 | 1:551:A:LYS:H    | 10       | 0.15          |
| (3,888) | 1:549:A:GLU:HB2 | 1:550:A:LYS:H    | 2        | 0.15          |
| (3,888) | 1:549:A:GLU:HB3 | 1:550:A:LYS:H    | 2        | 0.15          |
| (3,863) | 1:541:A:GLN:HA  | 1:541:A:GLN:HE21 | 2        | 0.15          |
| (3,863) | 1:541:A:GLN:HA  | 1:541:A:GLN:HE22 | 2        | 0.15          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD11 | 15       | 0.15          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD12 | 15       | 0.15          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD13 | 15       | 0.15          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD21 | 15       | 0.15          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD22 | 15       | 0.15          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD23 | 15       | 0.15          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD11 | 15       | 0.15          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD12 | 15       | 0.15          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD13 | 15       | 0.15          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD21 | 15       | 0.15          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD22 | 15       | 0.15          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD23 | 15       | 0.15          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG21 | 19       | 0.15          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG22 | 19       | 0.15          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG23 | 19       | 0.15          |
| (3,825) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HB   | 20       | 0.15          |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2  | 4        | 0.15          |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2  | 4        | 0.15          |
| (3,746) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HZ2  | 9        | 0.15          |
| (3,746) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HZ2  | 9        | 0.15          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 7        | 0.15          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 7        | 0.15          |
| (3,694) | 1:451:A:PHE:HZ   | 1:530:A:GLN:HA   | 16       | 0.15          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB2  | 4        | 0.15          |
| (3,685) | 1:525:A:SER:HA   | 1:529:A:GLU:HB3  | 4        | 0.15          |
| (3,647) | 1:458:A:LYS:H    | 1:524:A:LEU:H    | 6        | 0.15          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD11 | 14       | 0.15          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD12 | 14       | 0.15          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD13 | 14       | 0.15          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD21 | 14       | 0.15          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD22 | 14       | 0.15          |
| (3,626) | 1:521:A:LEU:H    | 1:521:A:LEU:HD23 | 14       | 0.15          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD11 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD12 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD13 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD21 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD22 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD23 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD11 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD12 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD13 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD21 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD22 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD23 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD11 | 16       | 0.15          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD12 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD13 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD21 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD22 | 16       | 0.15          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD23 | 16       | 0.15          |
| (3,585) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HE1  | 20       | 0.15          |
| (3,585) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HE1  | 20       | 0.15          |
| (3,585) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HE1  | 20       | 0.15          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 1        | 0.15          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 1        | 0.15          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 1        | 0.15          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 1        | 0.15          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 1        | 0.15          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 1        | 0.15          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 4        | 0.15          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 4        | 0.15          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 4        | 0.15          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 4        | 0.15          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 4        | 0.15          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 4        | 0.15          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 13       | 0.15          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 13       | 0.15          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 13       | 0.15          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 13       | 0.15          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 13       | 0.15          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 13       | 0.15          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 14       | 0.15          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 14       | 0.15          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 14       | 0.15          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 14       | 0.15          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 14       | 0.15          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 14       | 0.15          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 1        | 0.15          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 13       | 0.15          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 16       | 0.15          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB2  | 14       | 0.15          |
| (3,546) | 1:514:A:ASN:HD22 | 1:518:A:CYS:HB3  | 14       | 0.15          |
| (3,539) | 1:517:A:HIS:H    | 1:517:A:HIS:HD2  | 13       | 0.15          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE2  | 5        | 0.15          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE3  | 5        | 0.15          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE2  | 12       | 0.15          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE3  | 12       | 0.15          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE2  | 16       | 0.15          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE3  | 16       | 0.15          |
| (3,515) | 1:515:A:LYS:H    | 1:515:A:LYS:HG2  | 15       | 0.15          |
| (3,515) | 1:515:A:LYS:H    | 1:515:A:LYS:HG3  | 15       | 0.15          |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD21 | 20       | 0.15          |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD21 | 20       | 0.15          |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD22 | 20       | 0.15          |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD22 | 20       | 0.15          |
| (3,369) | 1:481:A:VAL:HG11 | 1:497:A:PHE:HD1  | 14       | 0.15          |
| (3,369) | 1:481:A:VAL:HG11 | 1:497:A:PHE:HD2  | 14       | 0.15          |
| (3,369) | 1:481:A:VAL:HG12 | 1:497:A:PHE:HD1  | 14       | 0.15          |
| (3,369) | 1:481:A:VAL:HG12 | 1:497:A:PHE:HD2  | 14       | 0.15          |
| (3,369) | 1:481:A:VAL:HG13 | 1:497:A:PHE:HD1  | 14       | 0.15          |
| (3,369) | 1:481:A:VAL:HG13 | 1:497:A:PHE:HD2  | 14       | 0.15          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 11       | 0.15          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 11       | 0.15          |
| (3,325) | 1:485:A:ASP:H    | 1:495:A:ALA:HA   | 17       | 0.15          |
| (3,303) | 1:459:A:ILE:HG12 | 1:494:A:HIS:HA   | 5        | 0.15          |
| (3,303) | 1:459:A:ILE:HG13 | 1:494:A:HIS:HA   | 5        | 0.15          |
| (3,280) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HA   | 15       | 0.15          |
| (3,280) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HA   | 15       | 0.15          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 11       | 0.15          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 11       | 0.15          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB2  | 11       | 0.15          |
| (3,279) | 1:486:A:LEU:HG   | 1:493:A:CYS:HB3  | 11       | 0.15          |
| (3,248) | 1:465:A:LEU:HD11 | 1:491:A:THR:HB   | 8        | 0.15          |
| (3,248) | 1:465:A:LEU:HD12 | 1:491:A:THR:HB   | 8        | 0.15          |
| (3,248) | 1:465:A:LEU:HD13 | 1:491:A:THR:HB   | 8        | 0.15          |
| (3,248) | 1:465:A:LEU:HD21 | 1:491:A:THR:HB   | 8        | 0.15          |
| (3,248) | 1:465:A:LEU:HD22 | 1:491:A:THR:HB   | 8        | 0.15          |
| (3,248) | 1:465:A:LEU:HD23 | 1:491:A:THR:HB   | 8        | 0.15          |
| (3,191) | 1:479:A:SER:HB2  | 1:481:A:VAL:HG11 | 6        | 0.15          |
| (3,191) | 1:479:A:SER:HB2  | 1:481:A:VAL:HG12 | 6        | 0.15          |
| (3,191) | 1:479:A:SER:HB2  | 1:481:A:VAL:HG13 | 6        | 0.15          |
| (3,191) | 1:479:A:SER:HB3  | 1:481:A:VAL:HG11 | 6        | 0.15          |
| (3,191) | 1:479:A:SER:HB3  | 1:481:A:VAL:HG12 | 6        | 0.15          |
| (3,191) | 1:479:A:SER:HB3  | 1:481:A:VAL:HG13 | 6        | 0.15          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD11 | 12       | 0.15          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD12 | 12       | 0.15          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD13 | 12       | 0.15          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD21 | 12       | 0.15          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD22 | 12       | 0.15          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD23 | 12       | 0.15          |
| (3,112) | 1:468:A:ARG:HG2 | 1:469:A:LYS:H    | 10       | 0.15          |
| (3,112) | 1:468:A:ARG:HG3 | 1:469:A:LYS:H    | 10       | 0.15          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD2  | 14       | 0.15          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD3  | 14       | 0.15          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD2  | 18       | 0.15          |
| (3,87)  | 1:463:A:GLU:H   | 1:464:A:PRO:HD3  | 18       | 0.15          |
| (3,17)  | 1:450:A:GLN:HA  | 1:451:A:PHE:HD1  | 3        | 0.15          |
| (3,17)  | 1:450:A:GLN:HA  | 1:451:A:PHE:HD2  | 3        | 0.15          |
| (1,43)  | 1:504:A:GLN:O   | 1:508:A:ASN:H    | 10       | 0.15          |
| (1,35)  | 1:500:A:PRO:O   | 1:504:A:GLN:H    | 20       | 0.15          |
| (1,13)  | 1:474:A:THR:O   | 1:478:A:ILE:H    | 19       | 0.15          |
| (3,902) | 1:555:A:GLU:H   | 1:555:A:GLU:HG2  | 17       | 0.14          |
| (3,902) | 1:555:A:GLU:H   | 1:555:A:GLU:HG3  | 17       | 0.14          |
| (3,888) | 1:549:A:GLU:HB2 | 1:550:A:LYS:H    | 4        | 0.14          |
| (3,888) | 1:549:A:GLU:HB3 | 1:550:A:LYS:H    | 4        | 0.14          |
| (3,872) | 1:545:A:ASN:H   | 1:545:A:ASN:HD21 | 7        | 0.14          |
| (3,872) | 1:545:A:ASN:H   | 1:545:A:ASN:HD22 | 7        | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD11 | 11       | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD12 | 11       | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD13 | 11       | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD21 | 11       | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD22 | 11       | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD23 | 11       | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD11 | 11       | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD12 | 11       | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD13 | 11       | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD21 | 11       | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD22 | 11       | 0.14          |
| (3,843) | 1:537:A:LEU:HA  | 1:537:A:LEU:HD23 | 11       | 0.14          |
| (3,827) | 1:533:A:TRP:HZ3 | 1:536:A:ILE:HG21 | 1        | 0.14          |
| (3,827) | 1:533:A:TRP:HZ3 | 1:536:A:ILE:HG22 | 1        | 0.14          |
| (3,827) | 1:533:A:TRP:HZ3 | 1:536:A:ILE:HG23 | 1        | 0.14          |
| (3,815) | 1:533:A:TRP:HA  | 1:536:A:ILE:HG12 | 17       | 0.14          |
| (3,815) | 1:533:A:TRP:HA  | 1:536:A:ILE:HG13 | 17       | 0.14          |
| (3,653) | 1:524:A:LEU:H   | 1:524:A:LEU:HG   | 18       | 0.14          |
| (3,621) | 1:510:A:TYR:HD1 | 1:521:A:LEU:HD11 | 10       | 0.14          |
| (3,621) | 1:510:A:TYR:HD1 | 1:521:A:LEU:HD12 | 10       | 0.14          |
| (3,621) | 1:510:A:TYR:HD1 | 1:521:A:LEU:HD13 | 10       | 0.14          |
| (3,621) | 1:510:A:TYR:HD1 | 1:521:A:LEU:HD21 | 10       | 0.14          |
| (3,621) | 1:510:A:TYR:HD1 | 1:521:A:LEU:HD22 | 10       | 0.14          |
| (3,621) | 1:510:A:TYR:HD1 | 1:521:A:LEU:HD23 | 10       | 0.14          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD11 | 10       | 0.14          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD12 | 10       | 0.14          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD13 | 10       | 0.14          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD21 | 10       | 0.14          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD22 | 10       | 0.14          |
| (3,621) | 1:510:A:TYR:HD1  | 1:521:A:LEU:HD23 | 10       | 0.14          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 2        | 0.14          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 2        | 0.14          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 2        | 0.14          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 2        | 0.14          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 2        | 0.14          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 2        | 0.14          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 5        | 0.14          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 5        | 0.14          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 5        | 0.14          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 5        | 0.14          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 5        | 0.14          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 5        | 0.14          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 11       | 0.14          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 11       | 0.14          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 11       | 0.14          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 11       | 0.14          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 11       | 0.14          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 11       | 0.14          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 18       | 0.14          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 18       | 0.14          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 18       | 0.14          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 18       | 0.14          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 18       | 0.14          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 18       | 0.14          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 3        | 0.14          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 6        | 0.14          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 9        | 0.14          |
| (3,561) | 1:461:A:SER:HB2  | 1:519:A:TRP:HD1  | 12       | 0.14          |
| (3,558) | 1:461:A:SER:HA   | 1:519:A:TRP:HD1  | 2        | 0.14          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE2  | 7        | 0.14          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE3  | 7        | 0.14          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE2  | 7        | 0.14          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE3  | 7        | 0.14          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE2  | 1        | 0.14          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE3  | 1        | 0.14          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE2  | 8        | 0.14          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE3  | 8        | 0.14          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE2  | 18       | 0.14          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE3  | 18       | 0.14          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 2        | 0.14          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 2        | 0.14          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 2        | 0.14          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE1  | 11       | 0.14          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE2  | 11       | 0.14          |
| (3,410) | 1:501:A:GLU:HG2  | 1:502:A:ASP:H    | 19       | 0.14          |
| (3,410) | 1:501:A:GLU:HG3  | 1:502:A:ASP:H    | 19       | 0.14          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB2  | 8        | 0.14          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB3  | 8        | 0.14          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB2  | 8        | 0.14          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB3  | 8        | 0.14          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB2  | 16       | 0.14          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB3  | 16       | 0.14          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB2  | 16       | 0.14          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB3  | 16       | 0.14          |
| (3,379) | 1:497:A:PHE:HB2  | 1:498:A:LYS:H    | 1        | 0.14          |
| (3,379) | 1:497:A:PHE:HB3  | 1:498:A:LYS:H    | 1        | 0.14          |
| (3,369) | 1:481:A:VAL:HG11 | 1:497:A:PHE:HD1  | 17       | 0.14          |
| (3,369) | 1:481:A:VAL:HG11 | 1:497:A:PHE:HD2  | 17       | 0.14          |
| (3,369) | 1:481:A:VAL:HG12 | 1:497:A:PHE:HD1  | 17       | 0.14          |
| (3,369) | 1:481:A:VAL:HG12 | 1:497:A:PHE:HD2  | 17       | 0.14          |
| (3,369) | 1:481:A:VAL:HG13 | 1:497:A:PHE:HD1  | 17       | 0.14          |
| (3,369) | 1:481:A:VAL:HG13 | 1:497:A:PHE:HD2  | 17       | 0.14          |
| (3,325) | 1:485:A:ASP:H    | 1:495:A:ALA:HA   | 18       | 0.14          |
| (3,308) | 1:492:A:GLU:HG2  | 1:494:A:HIS:HE1  | 7        | 0.14          |
| (3,308) | 1:492:A:GLU:HG3  | 1:494:A:HIS:HE1  | 7        | 0.14          |
| (3,280) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HA   | 18       | 0.14          |
| (3,280) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HA   | 18       | 0.14          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD11 | 2        | 0.14          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD12 | 2        | 0.14          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD13 | 2        | 0.14          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD21 | 2        | 0.14          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD22 | 2        | 0.14          |
| (3,234) | 1:487:A:LEU:HA   | 1:487:A:LEU:HD23 | 2        | 0.14          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD11 | 14       | 0.14          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD12 | 14       | 0.14          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD13 | 14       | 0.14          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD21 | 14       | 0.14          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD22 | 14       | 0.14          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD23 | 14       | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 2        | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 2        | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 2        | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 2        | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 2        | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 2        | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 18       | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 18       | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 18       | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 18       | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 18       | 0.14          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 18       | 0.14          |
| (3,113) | 1:469:A:LYS:H    | 1:469:A:LYS:HG2  | 14       | 0.14          |
| (3,113) | 1:469:A:LYS:H    | 1:469:A:LYS:HG3  | 14       | 0.14          |
| (3,112) | 1:468:A:ARG:HG2  | 1:469:A:LYS:H    | 4        | 0.14          |
| (3,112) | 1:468:A:ARG:HG3  | 1:469:A:LYS:H    | 4        | 0.14          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 19       | 0.14          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 19       | 0.14          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 19       | 0.14          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 19       | 0.14          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD2  | 7        | 0.14          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD3  | 7        | 0.14          |
| (3,52)  | 1:456:A:ILE:HG13 | 1:457:A:VAL:H    | 7        | 0.14          |
| (3,17)  | 1:450:A:GLN:HA   | 1:451:A:PHE:HD1  | 8        | 0.14          |
| (3,17)  | 1:450:A:GLN:HA   | 1:451:A:PHE:HD2  | 8        | 0.14          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE21 | 14       | 0.14          |
| (3,14)  | 1:450:A:GLN:HA   | 1:450:A:GLN:HE22 | 14       | 0.14          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG21 | 2        | 0.14          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG22 | 2        | 0.14          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG23 | 2        | 0.14          |
| (1,43)  | 1:504:A:GLN:O    | 1:508:A:ASN:H    | 3        | 0.14          |
| (1,37)  | 1:501:A:GLU:O    | 1:505:A:ALA:H    | 6        | 0.14          |
| (1,35)  | 1:500:A:PRO:O    | 1:504:A:GLN:H    | 7        | 0.14          |
| (1,13)  | 1:474:A:THR:O    | 1:478:A:ILE:H    | 2        | 0.14          |
| (1,13)  | 1:474:A:THR:O    | 1:478:A:ILE:H    | 7        | 0.14          |
| (1,13)  | 1:474:A:THR:O    | 1:478:A:ILE:H    | 11       | 0.14          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG12 | 18       | 0.13          |
| (3,910) | 1:558:A:ILE:H    | 1:558:A:ILE:HG13 | 18       | 0.13          |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG2  | 15       | 0.13          |
| (3,902) | 1:555:A:GLU:H    | 1:555:A:GLU:HG3  | 15       | 0.13          |
| (3,891) | 1:550:A:LYS:HG2  | 1:551:A:LYS:H    | 13       | 0.13          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,891) | 1:550:A:LYS:HG3  | 1:551:A:LYS:H    | 13       | 0.13          |
| (3,879) | 1:547:A:PRO:HB2  | 1:548:A:ARG:H    | 9        | 0.13          |
| (3,879) | 1:547:A:PRO:HB3  | 1:548:A:ARG:H    | 9        | 0.13          |
| (3,849) | 1:537:A:LEU:HB2  | 1:538:A:VAL:H    | 20       | 0.13          |
| (3,849) | 1:537:A:LEU:HB3  | 1:538:A:VAL:H    | 20       | 0.13          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD11 | 13       | 0.13          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD12 | 13       | 0.13          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD13 | 13       | 0.13          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD11 | 16       | 0.13          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD12 | 16       | 0.13          |
| (3,821) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HD13 | 16       | 0.13          |
| (3,749) | 1:496:A:ARG:HD2  | 1:533:A:TRP:HH2  | 15       | 0.13          |
| (3,749) | 1:496:A:ARG:HD3  | 1:533:A:TRP:HH2  | 15       | 0.13          |
| (3,733) | 1:451:A:PHE:HE1  | 1:533:A:TRP:HD1  | 7        | 0.13          |
| (3,733) | 1:451:A:PHE:HE2  | 1:533:A:TRP:HD1  | 7        | 0.13          |
| (3,731) | 1:451:A:PHE:HD1  | 1:533:A:TRP:HB3  | 7        | 0.13          |
| (3,731) | 1:451:A:PHE:HD2  | 1:533:A:TRP:HB3  | 7        | 0.13          |
| (3,720) | 1:524:A:LEU:HD11 | 1:532:A:TYR:HD2  | 8        | 0.13          |
| (3,720) | 1:524:A:LEU:HD12 | 1:532:A:TYR:HD2  | 8        | 0.13          |
| (3,720) | 1:524:A:LEU:HD13 | 1:532:A:TYR:HD2  | 8        | 0.13          |
| (3,720) | 1:524:A:LEU:HD21 | 1:532:A:TYR:HD2  | 8        | 0.13          |
| (3,720) | 1:524:A:LEU:HD22 | 1:532:A:TYR:HD2  | 8        | 0.13          |
| (3,720) | 1:524:A:LEU:HD23 | 1:532:A:TYR:HD2  | 8        | 0.13          |
| (3,706) | 1:530:A:GLN:HE21 | 1:531:A:ARG:HA   | 7        | 0.13          |
| (3,706) | 1:530:A:GLN:HE22 | 1:531:A:ARG:HA   | 7        | 0.13          |
| (3,694) | 1:451:A:PHE:HZ   | 1:530:A:GLN:HA   | 4        | 0.13          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB2  | 5        | 0.13          |
| (3,646) | 1:456:A:ILE:HG21 | 1:524:A:LEU:HB3  | 5        | 0.13          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB2  | 5        | 0.13          |
| (3,646) | 1:456:A:ILE:HG22 | 1:524:A:LEU:HB3  | 5        | 0.13          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB2  | 5        | 0.13          |
| (3,646) | 1:456:A:ILE:HG23 | 1:524:A:LEU:HB3  | 5        | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD11 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD12 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD13 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD21 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD22 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD23 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD11 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD12 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD13 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD21 | 9        | 0.13          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD22 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD23 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD11 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD12 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD13 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD21 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD22 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD23 | 9        | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD11 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD12 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD13 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD21 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD22 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG21 | 1:521:A:LEU:HD23 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD11 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD12 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD13 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD21 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD22 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG22 | 1:521:A:LEU:HD23 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD11 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD12 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD13 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD21 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD22 | 20       | 0.13          |
| (3,614) | 1:459:A:ILE:HG23 | 1:521:A:LEU:HD23 | 20       | 0.13          |
| (3,612) | 1:459:A:ILE:HG12 | 1:521:A:LEU:HA   | 4        | 0.13          |
| (3,612) | 1:459:A:ILE:HG13 | 1:521:A:LEU:HA   | 4        | 0.13          |
| (3,585) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HE1  | 7        | 0.13          |
| (3,585) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HE1  | 7        | 0.13          |
| (3,585) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HE1  | 7        | 0.13          |
| (3,585) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HE1  | 15       | 0.13          |
| (3,585) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HE1  | 15       | 0.13          |
| (3,585) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HE1  | 15       | 0.13          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 6        | 0.13          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 6        | 0.13          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 6        | 0.13          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 6        | 0.13          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 6        | 0.13          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 6        | 0.13          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 10       | 0.13          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 10       | 0.13          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 10       | 0.13          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 10       | 0.13          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 10       | 0.13          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 10       | 0.13          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 12       | 0.13          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 12       | 0.13          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 12       | 0.13          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 12       | 0.13          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 12       | 0.13          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 12       | 0.13          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 2        | 0.13          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 10       | 0.13          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 15       | 0.13          |
| (3,561) | 1:461:A:SER:HB2  | 1:519:A:TRP:HD1  | 1        | 0.13          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE2  | 7        | 0.13          |
| (3,522) | 1:516:A:LYS:HA   | 1:516:A:LYS:HE3  | 7        | 0.13          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 5        | 0.13          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 5        | 0.13          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 5        | 0.13          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE1  | 12       | 0.13          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE2  | 12       | 0.13          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE1  | 18       | 0.13          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE2  | 18       | 0.13          |
| (3,412) | 1:455:A:VAL:HG11 | 1:503:A:ALA:H    | 1        | 0.13          |
| (3,412) | 1:455:A:VAL:HG12 | 1:503:A:ALA:H    | 1        | 0.13          |
| (3,412) | 1:455:A:VAL:HG13 | 1:503:A:ALA:H    | 1        | 0.13          |
| (3,412) | 1:455:A:VAL:HG21 | 1:503:A:ALA:H    | 1        | 0.13          |
| (3,412) | 1:455:A:VAL:HG22 | 1:503:A:ALA:H    | 1        | 0.13          |
| (3,412) | 1:455:A:VAL:HG23 | 1:503:A:ALA:H    | 1        | 0.13          |
| (3,412) | 1:455:A:VAL:HG11 | 1:503:A:ALA:H    | 9        | 0.13          |
| (3,412) | 1:455:A:VAL:HG12 | 1:503:A:ALA:H    | 9        | 0.13          |
| (3,412) | 1:455:A:VAL:HG13 | 1:503:A:ALA:H    | 9        | 0.13          |
| (3,412) | 1:455:A:VAL:HG21 | 1:503:A:ALA:H    | 9        | 0.13          |
| (3,412) | 1:455:A:VAL:HG22 | 1:503:A:ALA:H    | 9        | 0.13          |
| (3,412) | 1:455:A:VAL:HG23 | 1:503:A:ALA:H    | 9        | 0.13          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG2  | 1        | 0.13          |
| (3,395) | 1:499:A:THR:HB   | 1:501:A:GLU:HG3  | 1        | 0.13          |
| (3,379) | 1:497:A:PHE:HB2  | 1:498:A:LYS:H    | 2        | 0.13          |
| (3,379) | 1:497:A:PHE:HB3  | 1:498:A:LYS:H    | 2        | 0.13          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG2  | 10       | 0.13          |
| (3,351) | 1:496:A:ARG:H    | 1:496:A:ARG:HG3  | 10       | 0.13          |
| (3,347) | 1:485:A:ASP:H    | 1:496:A:ARG:H    | 9        | 0.13          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (3,347) | 1:485:A:ASP:H   | 1:496:A:ARG:H    | 10       | 0.13          |
| (3,323) | 1:484:A:VAL:HA  | 1:495:A:ALA:HB1  | 6        | 0.13          |
| (3,323) | 1:484:A:VAL:HA  | 1:495:A:ALA:HB2  | 6        | 0.13          |
| (3,323) | 1:484:A:VAL:HA  | 1:495:A:ALA:HB3  | 6        | 0.13          |
| (3,323) | 1:484:A:VAL:HA  | 1:495:A:ALA:HB1  | 16       | 0.13          |
| (3,323) | 1:484:A:VAL:HA  | 1:495:A:ALA:HB2  | 16       | 0.13          |
| (3,323) | 1:484:A:VAL:HA  | 1:495:A:ALA:HB3  | 16       | 0.13          |
| (3,201) | 1:482:A:LEU:HB2 | 1:483:A:TYR:HB2  | 2        | 0.13          |
| (3,201) | 1:482:A:LEU:HB2 | 1:483:A:TYR:HB3  | 2        | 0.13          |
| (3,201) | 1:482:A:LEU:HB3 | 1:483:A:TYR:HB2  | 2        | 0.13          |
| (3,201) | 1:482:A:LEU:HB3 | 1:483:A:TYR:HB3  | 2        | 0.13          |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD11 | 5        | 0.13          |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD12 | 5        | 0.13          |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD13 | 5        | 0.13          |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD21 | 5        | 0.13          |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD22 | 5        | 0.13          |
| (3,162) | 1:475:A:LEU:H   | 1:475:A:LEU:HD23 | 5        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG11 | 3        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG12 | 3        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG13 | 3        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG21 | 3        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG22 | 3        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG23 | 3        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG11 | 4        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG12 | 4        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG13 | 4        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG21 | 4        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG22 | 4        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG23 | 4        | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG11 | 13       | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG12 | 13       | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG13 | 13       | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG21 | 13       | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG22 | 13       | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG23 | 13       | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG11 | 15       | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG12 | 15       | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG13 | 15       | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG21 | 15       | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG22 | 15       | 0.13          |
| (3,131) | 1:471:A:VAL:H   | 1:471:A:VAL:HG23 | 15       | 0.13          |
| (3,113) | 1:469:A:LYS:H   | 1:469:A:LYS:HG2  | 9        | 0.13          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,113) | 1:469:A:LYS:H    | 1:469:A:LYS:HG3  | 9        | 0.13          |
| (3,112) | 1:468:A:ARG:HG2  | 1:469:A:LYS:H    | 6        | 0.13          |
| (3,112) | 1:468:A:ARG:HG3  | 1:469:A:LYS:H    | 6        | 0.13          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 5        | 0.13          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 5        | 0.13          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 5        | 0.13          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 5        | 0.13          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD2  | 1        | 0.13          |
| (3,87)  | 1:463:A:GLU:H    | 1:464:A:PRO:HD3  | 1        | 0.13          |
| (3,83)  | 1:462:A:THR:H    | 1:463:A:GLU:HB2  | 16       | 0.13          |
| (3,83)  | 1:462:A:THR:H    | 1:463:A:GLU:HB3  | 16       | 0.13          |
| (3,52)  | 1:456:A:ILE:HG13 | 1:457:A:VAL:H    | 6        | 0.13          |
| (3,34)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:HA2  | 15       | 0.13          |
| (3,34)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:HA3  | 15       | 0.13          |
| (3,34)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:HA2  | 15       | 0.13          |
| (3,34)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:HA3  | 15       | 0.13          |
| (3,34)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:HA2  | 15       | 0.13          |
| (3,34)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:HA3  | 15       | 0.13          |
| (3,34)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:HA2  | 15       | 0.13          |
| (3,34)  | 1:452:A:VAL:HG21 | 1:454:A:GLY:HA3  | 15       | 0.13          |
| (3,34)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:HA2  | 15       | 0.13          |
| (3,34)  | 1:452:A:VAL:HG22 | 1:454:A:GLY:HA3  | 15       | 0.13          |
| (3,34)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:HA2  | 15       | 0.13          |
| (3,34)  | 1:452:A:VAL:HG23 | 1:454:A:GLY:HA3  | 15       | 0.13          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG21 | 8        | 0.13          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG22 | 8        | 0.13          |
| (3,7)   | 1:447:A:THR:H    | 1:447:A:THR:HG23 | 8        | 0.13          |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 9        | 0.13          |
| (1,71)  | 1:531:A:ARG:O    | 1:535:A:LYS:H    | 1        | 0.13          |
| (1,71)  | 1:531:A:ARG:O    | 1:535:A:LYS:H    | 14       | 0.13          |
| (1,71)  | 1:531:A:ARG:O    | 1:535:A:LYS:H    | 17       | 0.13          |
| (1,45)  | 1:505:A:ALA:O    | 1:509:A:ALA:H    | 12       | 0.13          |
| (1,43)  | 1:504:A:GLN:O    | 1:508:A:ASN:H    | 18       | 0.13          |
| (1,40)  | 1:502:A:ASP:O    | 1:506:A:VAL:N    | 12       | 0.13          |
| (1,36)  | 1:500:A:PRO:O    | 1:504:A:GLN:N    | 18       | 0.13          |
| (1,13)  | 1:474:A:THR:O    | 1:478:A:ILE:H    | 16       | 0.13          |
| (1,13)  | 1:474:A:THR:O    | 1:478:A:ILE:H    | 20       | 0.13          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD11 | 18       | 0.12          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD12 | 18       | 0.12          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD13 | 18       | 0.12          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD21 | 18       | 0.12          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD22 | 18       | 0.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD23 | 18       | 0.12          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD11 | 18       | 0.12          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD12 | 18       | 0.12          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD13 | 18       | 0.12          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD21 | 18       | 0.12          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD22 | 18       | 0.12          |
| (3,843) | 1:537:A:LEU:HA   | 1:537:A:LEU:HD23 | 18       | 0.12          |
| (3,842) | 1:536:A:ILE:HG21 | 1:537:A:LEU:H    | 3        | 0.12          |
| (3,842) | 1:536:A:ILE:HG22 | 1:537:A:LEU:H    | 3        | 0.12          |
| (3,842) | 1:536:A:ILE:HG23 | 1:537:A:LEU:H    | 3        | 0.12          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG21 | 17       | 0.12          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG22 | 17       | 0.12          |
| (3,827) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HG23 | 17       | 0.12          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD11 | 7        | 0.12          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD12 | 7        | 0.12          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD13 | 7        | 0.12          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 11       | 0.12          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 11       | 0.12          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG12 | 15       | 0.12          |
| (3,815) | 1:533:A:TRP:HA   | 1:536:A:ILE:HG13 | 15       | 0.12          |
| (3,808) | 1:532:A:TYR:HD1  | 1:536:A:ILE:HD11 | 13       | 0.12          |
| (3,808) | 1:532:A:TYR:HD1  | 1:536:A:ILE:HD12 | 13       | 0.12          |
| (3,808) | 1:532:A:TYR:HD1  | 1:536:A:ILE:HD13 | 13       | 0.12          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD11 | 11       | 0.12          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD12 | 11       | 0.12          |
| (3,802) | 1:496:A:ARG:HD3  | 1:536:A:ILE:HD13 | 11       | 0.12          |
| (3,747) | 1:496:A:ARG:HB2  | 1:533:A:TRP:HH2  | 1        | 0.12          |
| (3,747) | 1:496:A:ARG:HB3  | 1:533:A:TRP:HH2  | 1        | 0.12          |
| (3,689) | 1:526:A:GLY:H    | 1:529:A:GLU:HG2  | 12       | 0.12          |
| (3,689) | 1:526:A:GLY:H    | 1:529:A:GLU:HG3  | 12       | 0.12          |
| (3,653) | 1:524:A:LEU:H    | 1:524:A:LEU:HG   | 14       | 0.12          |
| (3,585) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HE1  | 2        | 0.12          |
| (3,585) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HE1  | 2        | 0.12          |
| (3,585) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HE1  | 2        | 0.12          |
| (3,579) | 1:471:A:VAL:HG11 | 1:519:A:TRP:HZ2  | 3        | 0.12          |
| (3,579) | 1:471:A:VAL:HG12 | 1:519:A:TRP:HZ2  | 3        | 0.12          |
| (3,579) | 1:471:A:VAL:HG13 | 1:519:A:TRP:HZ2  | 3        | 0.12          |
| (3,579) | 1:471:A:VAL:HG21 | 1:519:A:TRP:HZ2  | 3        | 0.12          |
| (3,579) | 1:471:A:VAL:HG22 | 1:519:A:TRP:HZ2  | 3        | 0.12          |
| (3,579) | 1:471:A:VAL:HG23 | 1:519:A:TRP:HZ2  | 3        | 0.12          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 12       | 0.12          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 17       | 0.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE2  | 11       | 0.12          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE3  | 11       | 0.12          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE2  | 11       | 0.12          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE3  | 11       | 0.12          |
| (3,515) | 1:515:A:LYS:H    | 1:515:A:LYS:HG2  | 14       | 0.12          |
| (3,515) | 1:515:A:LYS:H    | 1:515:A:LYS:HG3  | 14       | 0.12          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 3        | 0.12          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 3        | 0.12          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 3        | 0.12          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE1  | 1        | 0.12          |
| (3,469) | 1:475:A:LEU:HA   | 1:510:A:TYR:HE2  | 1        | 0.12          |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD21 | 12       | 0.12          |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD21 | 12       | 0.12          |
| (3,459) | 1:507:A:ILE:HG12 | 1:508:A:ASN:HD22 | 12       | 0.12          |
| (3,459) | 1:507:A:ILE:HG13 | 1:508:A:ASN:HD22 | 12       | 0.12          |
| (3,447) | 1:504:A:GLN:HG2  | 1:508:A:ASN:HD21 | 16       | 0.12          |
| (3,447) | 1:504:A:GLN:HG3  | 1:508:A:ASN:HD21 | 16       | 0.12          |
| (3,447) | 1:504:A:GLN:HG2  | 1:508:A:ASN:HD22 | 16       | 0.12          |
| (3,447) | 1:504:A:GLN:HG3  | 1:508:A:ASN:HD22 | 16       | 0.12          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD21 | 2        | 0.12          |
| (3,446) | 1:504:A:GLN:HB2  | 1:508:A:ASN:HD22 | 2        | 0.12          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD21 | 2        | 0.12          |
| (3,446) | 1:504:A:GLN:HB3  | 1:508:A:ASN:HD22 | 2        | 0.12          |
| (3,412) | 1:455:A:VAL:HG11 | 1:503:A:ALA:H    | 11       | 0.12          |
| (3,412) | 1:455:A:VAL:HG12 | 1:503:A:ALA:H    | 11       | 0.12          |
| (3,412) | 1:455:A:VAL:HG13 | 1:503:A:ALA:H    | 11       | 0.12          |
| (3,412) | 1:455:A:VAL:HG21 | 1:503:A:ALA:H    | 11       | 0.12          |
| (3,412) | 1:455:A:VAL:HG22 | 1:503:A:ALA:H    | 11       | 0.12          |
| (3,412) | 1:455:A:VAL:HG23 | 1:503:A:ALA:H    | 11       | 0.12          |
| (3,325) | 1:485:A:ASP:H    | 1:495:A:ALA:HA   | 7        | 0.12          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB1  | 10       | 0.12          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB2  | 10       | 0.12          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB3  | 10       | 0.12          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB1  | 18       | 0.12          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB2  | 18       | 0.12          |
| (3,323) | 1:484:A:VAL:HA   | 1:495:A:ALA:HB3  | 18       | 0.12          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB2  | 10       | 0.12          |
| (3,281) | 1:486:A:LEU:HB2  | 1:493:A:CYS:HB3  | 10       | 0.12          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB2  | 10       | 0.12          |
| (3,281) | 1:486:A:LEU:HB3  | 1:493:A:CYS:HB3  | 10       | 0.12          |
| (3,261) | 1:491:A:THR:H    | 1:492:A:GLU:HG2  | 17       | 0.12          |
| (3,261) | 1:491:A:THR:H    | 1:492:A:GLU:HG3  | 17       | 0.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,237) | 1:488:A:GLU:H    | 1:488:A:GLU:HB2  | 9        | 0.12          |
| (3,237) | 1:488:A:GLU:H    | 1:488:A:GLU:HB3  | 9        | 0.12          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD11 | 10       | 0.12          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD12 | 10       | 0.12          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD13 | 10       | 0.12          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD21 | 10       | 0.12          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD22 | 10       | 0.12          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD23 | 10       | 0.12          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 5        | 0.12          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 5        | 0.12          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 5        | 0.12          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 5        | 0.12          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 5        | 0.12          |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 5        | 0.12          |
| (3,112) | 1:468:A:ARG:HG2  | 1:469:A:LYS:H    | 14       | 0.12          |
| (3,112) | 1:468:A:ARG:HG3  | 1:469:A:LYS:H    | 14       | 0.12          |
| (3,52)  | 1:456:A:ILE:HG13 | 1:457:A:VAL:H    | 12       | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 7        | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 7        | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 7        | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 7        | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 7        | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 7        | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 9        | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 9        | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 9        | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 9        | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 9        | 0.12          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 9        | 0.12          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB2  | 9        | 0.12          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB2  | 9        | 0.12          |
| (3,30)  | 1:451:A:PHE:HE1  | 1:453:A:SER:HB3  | 9        | 0.12          |
| (3,30)  | 1:451:A:PHE:HE2  | 1:453:A:SER:HB3  | 9        | 0.12          |
| (1,71)  | 1:531:A:ARG:O    | 1:535:A:LYS:H    | 10       | 0.12          |
| (1,35)  | 1:500:A:PRO:O    | 1:504:A:GLN:H    | 4        | 0.12          |
| (1,35)  | 1:500:A:PRO:O    | 1:504:A:GLN:H    | 13       | 0.12          |
| (1,13)  | 1:474:A:THR:O    | 1:478:A:ILE:H    | 12       | 0.12          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD11 | 19       | 0.11          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD12 | 19       | 0.11          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD13 | 19       | 0.11          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD21 | 19       | 0.11          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD22 | 19       | 0.11          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD23 | 19       | 0.11          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD11 | 19       | 0.11          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD12 | 19       | 0.11          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD13 | 19       | 0.11          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD21 | 19       | 0.11          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD22 | 19       | 0.11          |
| (3,907) | 1:557:A:LEU:HA   | 1:557:A:LEU:HD23 | 19       | 0.11          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD21 | 8        | 0.11          |
| (3,872) | 1:545:A:ASN:H    | 1:545:A:ASN:HD22 | 8        | 0.11          |
| (3,849) | 1:537:A:LEU:HB2  | 1:538:A:VAL:H    | 19       | 0.11          |
| (3,849) | 1:537:A:LEU:HB3  | 1:538:A:VAL:H    | 19       | 0.11          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD11 | 19       | 0.11          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD12 | 19       | 0.11          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD13 | 19       | 0.11          |
| (3,822) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HG12 | 20       | 0.11          |
| (3,822) | 1:533:A:TRP:HE3  | 1:536:A:ILE:HG13 | 20       | 0.11          |
| (3,797) | 1:535:A:LYS:HB2  | 1:535:A:LYS:HE2  | 15       | 0.11          |
| (3,797) | 1:535:A:LYS:HB2  | 1:535:A:LYS:HE3  | 15       | 0.11          |
| (3,797) | 1:535:A:LYS:HB3  | 1:535:A:LYS:HE2  | 15       | 0.11          |
| (3,797) | 1:535:A:LYS:HB3  | 1:535:A:LYS:HE3  | 15       | 0.11          |
| (3,731) | 1:451:A:PHE:HD1  | 1:533:A:TRP:HB3  | 16       | 0.11          |
| (3,731) | 1:451:A:PHE:HD2  | 1:533:A:TRP:HB3  | 16       | 0.11          |
| (3,725) | 1:531:A:ARG:HD2  | 1:532:A:TYR:H    | 5        | 0.11          |
| (3,725) | 1:531:A:ARG:HD3  | 1:532:A:TYR:H    | 5        | 0.11          |
| (3,705) | 1:530:A:GLN:HE21 | 1:531:A:ARG:H    | 12       | 0.11          |
| (3,705) | 1:530:A:GLN:HE22 | 1:531:A:ARG:H    | 12       | 0.11          |
| (3,694) | 1:451:A:PHE:HZ   | 1:530:A:GLN:HA   | 15       | 0.11          |
| (3,694) | 1:451:A:PHE:HZ   | 1:530:A:GLN:HA   | 18       | 0.11          |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD2  | 5        | 0.11          |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD3  | 5        | 0.11          |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD2  | 11       | 0.11          |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD3  | 11       | 0.11          |
| (3,598) | 1:519:A:TRP:HE1  | 1:520:A:LYS:HB2  | 7        | 0.11          |
| (3,598) | 1:519:A:TRP:HE1  | 1:520:A:LYS:HB3  | 7        | 0.11          |
| (3,598) | 1:519:A:TRP:HE1  | 1:520:A:LYS:HB2  | 20       | 0.11          |
| (3,598) | 1:519:A:TRP:HE1  | 1:520:A:LYS:HB3  | 20       | 0.11          |
| (3,585) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HE1  | 19       | 0.11          |
| (3,585) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HE1  | 19       | 0.11          |
| (3,585) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HE1  | 19       | 0.11          |
| (3,576) | 1:471:A:VAL:HA   | 1:519:A:TRP:HH2  | 5        | 0.11          |
| (3,556) | 1:460:A:ILE:HG21 | 1:519:A:TRP:HA   | 9        | 0.11          |
| (3,556) | 1:460:A:ILE:HG22 | 1:519:A:TRP:HA   | 9        | 0.11          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,556) | 1:460:A:ILE:HG23 | 1:519:A:TRP:HA   | 9        | 0.11          |
| (3,556) | 1:460:A:ILE:HG21 | 1:519:A:TRP:HA   | 10       | 0.11          |
| (3,556) | 1:460:A:ILE:HG22 | 1:519:A:TRP:HA   | 10       | 0.11          |
| (3,556) | 1:460:A:ILE:HG23 | 1:519:A:TRP:HA   | 10       | 0.11          |
| (3,556) | 1:460:A:ILE:HG21 | 1:519:A:TRP:HA   | 12       | 0.11          |
| (3,556) | 1:460:A:ILE:HG22 | 1:519:A:TRP:HA   | 12       | 0.11          |
| (3,556) | 1:460:A:ILE:HG23 | 1:519:A:TRP:HA   | 12       | 0.11          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE2  | 16       | 0.11          |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE3  | 16       | 0.11          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE2  | 16       | 0.11          |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE3  | 16       | 0.11          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD11 | 11       | 0.11          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD12 | 11       | 0.11          |
| (3,497) | 1:513:A:ILE:HA   | 1:513:A:ILE:HD13 | 11       | 0.11          |
| (3,490) | 1:510:A:TYR:HD2  | 1:512:A:GLU:H    | 2        | 0.11          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG21 | 15       | 0.11          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG22 | 15       | 0.11          |
| (3,487) | 1:511:A:THR:H    | 1:511:A:THR:HG23 | 15       | 0.11          |
| (3,456) | 1:507:A:ILE:HD11 | 1:508:A:ASN:H    | 3        | 0.11          |
| (3,456) | 1:507:A:ILE:HD12 | 1:508:A:ASN:H    | 3        | 0.11          |
| (3,456) | 1:507:A:ILE:HD13 | 1:508:A:ASN:H    | 3        | 0.11          |
| (3,439) | 1:503:A:ALA:HA   | 1:506:A:VAL:HG11 | 7        | 0.11          |
| (3,439) | 1:503:A:ALA:HA   | 1:506:A:VAL:HG12 | 7        | 0.11          |
| (3,439) | 1:503:A:ALA:HA   | 1:506:A:VAL:HG13 | 7        | 0.11          |
| (3,439) | 1:503:A:ALA:HA   | 1:506:A:VAL:HG21 | 7        | 0.11          |
| (3,439) | 1:503:A:ALA:HA   | 1:506:A:VAL:HG22 | 7        | 0.11          |
| (3,439) | 1:503:A:ALA:HA   | 1:506:A:VAL:HG23 | 7        | 0.11          |
| (3,412) | 1:455:A:VAL:HG11 | 1:503:A:ALA:H    | 8        | 0.11          |
| (3,412) | 1:455:A:VAL:HG12 | 1:503:A:ALA:H    | 8        | 0.11          |
| (3,412) | 1:455:A:VAL:HG13 | 1:503:A:ALA:H    | 8        | 0.11          |
| (3,412) | 1:455:A:VAL:HG21 | 1:503:A:ALA:H    | 8        | 0.11          |
| (3,412) | 1:455:A:VAL:HG22 | 1:503:A:ALA:H    | 8        | 0.11          |
| (3,412) | 1:455:A:VAL:HG23 | 1:503:A:ALA:H    | 8        | 0.11          |
| (3,410) | 1:501:A:GLU:HG2  | 1:502:A:ASP:H    | 2        | 0.11          |
| (3,410) | 1:501:A:GLU:HG3  | 1:502:A:ASP:H    | 2        | 0.11          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB2  | 20       | 0.11          |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB3  | 20       | 0.11          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB2  | 20       | 0.11          |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB3  | 20       | 0.11          |
| (3,379) | 1:497:A:PHE:HB2  | 1:498:A:LYS:H    | 8        | 0.11          |
| (3,379) | 1:497:A:PHE:HB3  | 1:498:A:LYS:H    | 8        | 0.11          |
| (3,333) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HA   | 12       | 0.11          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,333) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HA   | 12       | 0.11          |
| (3,333) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HA   | 12       | 0.11          |
| (3,277) | 1:486:A:LEU:HA   | 1:493:A:CYS:HA   | 17       | 0.11          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB2  | 15       | 0.11          |
| (3,201) | 1:482:A:LEU:HB2  | 1:483:A:TYR:HB3  | 15       | 0.11          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB2  | 15       | 0.11          |
| (3,201) | 1:482:A:LEU:HB3  | 1:483:A:TYR:HB3  | 15       | 0.11          |
| (3,179) | 1:478:A:ILE:HA   | 1:478:A:ILE:HG12 | 4        | 0.11          |
| (3,179) | 1:478:A:ILE:HA   | 1:478:A:ILE:HG13 | 4        | 0.11          |
| (3,179) | 1:478:A:ILE:HA   | 1:478:A:ILE:HG12 | 9        | 0.11          |
| (3,179) | 1:478:A:ILE:HA   | 1:478:A:ILE:HG13 | 9        | 0.11          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD11 | 2        | 0.11          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD12 | 2        | 0.11          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD13 | 2        | 0.11          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD21 | 2        | 0.11          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD22 | 2        | 0.11          |
| (3,162) | 1:475:A:LEU:H    | 1:475:A:LEU:HD23 | 2        | 0.11          |
| (3,112) | 1:468:A:ARG:HG2  | 1:469:A:LYS:H    | 18       | 0.11          |
| (3,112) | 1:468:A:ARG:HG3  | 1:469:A:LYS:H    | 18       | 0.11          |
| (3,103) | 1:466:A:PRO:HD2  | 1:467:A:GLY:H    | 7        | 0.11          |
| (3,103) | 1:466:A:PRO:HD3  | 1:467:A:GLY:H    | 7        | 0.11          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB2  | 6        | 0.11          |
| (3,94)  | 1:461:A:SER:HB2  | 1:465:A:LEU:HB3  | 6        | 0.11          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB2  | 6        | 0.11          |
| (3,94)  | 1:461:A:SER:HB3  | 1:465:A:LEU:HB3  | 6        | 0.11          |
| (3,79)  | 1:461:A:SER:HB2  | 1:462:A:THR:H    | 18       | 0.11          |
| (3,79)  | 1:461:A:SER:HB3  | 1:462:A:THR:H    | 18       | 0.11          |
| (3,52)  | 1:456:A:ILE:HG13 | 1:457:A:VAL:H    | 16       | 0.11          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 13       | 0.11          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 13       | 0.11          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 13       | 0.11          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 13       | 0.11          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 13       | 0.11          |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 13       | 0.11          |
| (3,6)   | 1:446:A:ALA:HB1  | 1:447:A:THR:H    | 20       | 0.11          |
| (3,6)   | 1:446:A:ALA:HB2  | 1:447:A:THR:H    | 20       | 0.11          |
| (3,6)   | 1:446:A:ALA:HB3  | 1:447:A:THR:H    | 20       | 0.11          |
| (3,3)   | 1:445:A:ASN:HB3  | 1:446:A:ALA:H    | 3        | 0.11          |
| (1,73)  | 1:532:A:TYR:O    | 1:536:A:ILE:H    | 8        | 0.11          |
| (1,71)  | 1:531:A:ARG:O    | 1:535:A:LYS:H    | 3        | 0.11          |
| (1,13)  | 1:474:A:THR:O    | 1:478:A:ILE:H    | 4        | 0.11          |
| (1,13)  | 1:474:A:THR:O    | 1:478:A:ILE:H    | 13       | 0.11          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,13)  | 1:474:A:THR:O    | 1:478:A:ILE:H    | 14       | 0.11          |
| (1,7)   | 1:471:A:VAL:O    | 1:475:A:LEU:H    | 6        | 0.11          |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD11 | 20       | 0.1           |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD12 | 20       | 0.1           |
| (3,826) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HD13 | 20       | 0.1           |
| (3,825) | 1:533:A:TRP:HZ3  | 1:536:A:ILE:HB   | 9        | 0.1           |
| (3,730) | 1:451:A:PHE:HZ   | 1:533:A:TRP:HD1  | 10       | 0.1           |
| (3,696) | 1:525:A:SER:HA   | 1:530:A:GLN:H    | 16       | 0.1           |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD2  | 2        | 0.1           |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD3  | 2        | 0.1           |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD2  | 4        | 0.1           |
| (3,606) | 1:520:A:LYS:HA   | 1:520:A:LYS:HD3  | 4        | 0.1           |
| (3,598) | 1:519:A:TRP:HE1  | 1:520:A:LYS:HB2  | 8        | 0.1           |
| (3,598) | 1:519:A:TRP:HE1  | 1:520:A:LYS:HB3  | 8        | 0.1           |
| (3,585) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HE1  | 1        | 0.1           |
| (3,585) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HE1  | 1        | 0.1           |
| (3,585) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HE1  | 1        | 0.1           |
| (3,585) | 1:513:A:ILE:HG21 | 1:519:A:TRP:HE1  | 17       | 0.1           |
| (3,585) | 1:513:A:ILE:HG22 | 1:519:A:TRP:HE1  | 17       | 0.1           |
| (3,585) | 1:513:A:ILE:HG23 | 1:519:A:TRP:HE1  | 17       | 0.1           |
| (3,556) | 1:460:A:ILE:HG21 | 1:519:A:TRP:HA   | 8        | 0.1           |
| (3,556) | 1:460:A:ILE:HG22 | 1:519:A:TRP:HA   | 8        | 0.1           |
| (3,556) | 1:460:A:ILE:HG23 | 1:519:A:TRP:HA   | 8        | 0.1           |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE2  | 12       | 0.1           |
| (3,525) | 1:516:A:LYS:HG2  | 1:516:A:LYS:HE3  | 12       | 0.1           |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE2  | 12       | 0.1           |
| (3,525) | 1:516:A:LYS:HG3  | 1:516:A:LYS:HE3  | 12       | 0.1           |
| (3,489) | 1:510:A:TYR:HB3  | 1:512:A:GLU:H    | 5        | 0.1           |
| (3,489) | 1:510:A:TYR:HB3  | 1:512:A:GLU:H    | 6        | 0.1           |
| (3,489) | 1:510:A:TYR:HB3  | 1:512:A:GLU:H    | 17       | 0.1           |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB2  | 14       | 0.1           |
| (3,401) | 1:497:A:PHE:HD1  | 1:502:A:ASP:HB3  | 14       | 0.1           |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB2  | 14       | 0.1           |
| (3,401) | 1:497:A:PHE:HD2  | 1:502:A:ASP:HB3  | 14       | 0.1           |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD2  | 4        | 0.1           |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD2  | 4        | 0.1           |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD2  | 4        | 0.1           |
| (3,335) | 1:456:A:ILE:HD11 | 1:496:A:ARG:HD3  | 4        | 0.1           |
| (3,335) | 1:456:A:ILE:HD12 | 1:496:A:ARG:HD3  | 4        | 0.1           |
| (3,335) | 1:456:A:ILE:HD13 | 1:496:A:ARG:HD3  | 4        | 0.1           |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 13       | 0.1           |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 13       | 0.1           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 13       | 0.1           |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 13       | 0.1           |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 13       | 0.1           |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 13       | 0.1           |
| (3,247) | 1:465:A:LEU:HD11 | 1:491:A:THR:HA   | 13       | 0.1           |
| (3,247) | 1:465:A:LEU:HD12 | 1:491:A:THR:HA   | 13       | 0.1           |
| (3,247) | 1:465:A:LEU:HD13 | 1:491:A:THR:HA   | 13       | 0.1           |
| (3,247) | 1:465:A:LEU:HD21 | 1:491:A:THR:HA   | 13       | 0.1           |
| (3,247) | 1:465:A:LEU:HD22 | 1:491:A:THR:HA   | 13       | 0.1           |
| (3,247) | 1:465:A:LEU:HD23 | 1:491:A:THR:HA   | 13       | 0.1           |
| (3,237) | 1:488:A:GLU:H    | 1:488:A:GLU:HB2  | 16       | 0.1           |
| (3,237) | 1:488:A:GLU:H    | 1:488:A:GLU:HB3  | 16       | 0.1           |
| (3,237) | 1:488:A:GLU:H    | 1:488:A:GLU:HB2  | 20       | 0.1           |
| (3,237) | 1:488:A:GLU:H    | 1:488:A:GLU:HB3  | 20       | 0.1           |
| (3,207) | 1:472:A:ARG:HA   | 1:484:A:VAL:HG11 | 7        | 0.1           |
| (3,207) | 1:472:A:ARG:HA   | 1:484:A:VAL:HG12 | 7        | 0.1           |
| (3,207) | 1:472:A:ARG:HA   | 1:484:A:VAL:HG13 | 7        | 0.1           |
| (3,207) | 1:472:A:ARG:HA   | 1:484:A:VAL:HG21 | 7        | 0.1           |
| (3,207) | 1:472:A:ARG:HA   | 1:484:A:VAL:HG22 | 7        | 0.1           |
| (3,207) | 1:472:A:ARG:HA   | 1:484:A:VAL:HG23 | 7        | 0.1           |
| (3,179) | 1:478:A:ILE:HA   | 1:478:A:ILE:HG12 | 13       | 0.1           |
| (3,179) | 1:478:A:ILE:HA   | 1:478:A:ILE:HG13 | 13       | 0.1           |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG11 | 1        | 0.1           |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG12 | 1        | 0.1           |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG13 | 1        | 0.1           |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG21 | 1        | 0.1           |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG22 | 1        | 0.1           |
| (3,131) | 1:471:A:VAL:H    | 1:471:A:VAL:HG23 | 1        | 0.1           |
| (3,112) | 1:468:A:ARG:HG2  | 1:469:A:LYS:H    | 16       | 0.1           |
| (3,112) | 1:468:A:ARG:HG3  | 1:469:A:LYS:H    | 16       | 0.1           |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG11 | 5        | 0.1           |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG12 | 5        | 0.1           |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG13 | 5        | 0.1           |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG21 | 5        | 0.1           |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG22 | 5        | 0.1           |
| (3,37)  | 1:455:A:VAL:H    | 1:455:A:VAL:HG23 | 5        | 0.1           |
| (3,34)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:HA2  | 18       | 0.1           |
| (3,34)  | 1:452:A:VAL:HG11 | 1:454:A:GLY:HA3  | 18       | 0.1           |
| (3,34)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:HA2  | 18       | 0.1           |
| (3,34)  | 1:452:A:VAL:HG12 | 1:454:A:GLY:HA3  | 18       | 0.1           |
| (3,34)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:HA2  | 18       | 0.1           |
| (3,34)  | 1:452:A:VAL:HG13 | 1:454:A:GLY:HA3  | 18       | 0.1           |

*Continued on next page...*

*Continued from previous page...*

| Key    | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|--------|------------------|-----------------|----------|---------------|
| (3,34) | 1:452:A:VAL:HG21 | 1:454:A:GLY:HA2 | 18       | 0.1           |
| (3,34) | 1:452:A:VAL:HG21 | 1:454:A:GLY:HA3 | 18       | 0.1           |
| (3,34) | 1:452:A:VAL:HG22 | 1:454:A:GLY:HA2 | 18       | 0.1           |
| (3,34) | 1:452:A:VAL:HG22 | 1:454:A:GLY:HA3 | 18       | 0.1           |
| (3,34) | 1:452:A:VAL:HG23 | 1:454:A:GLY:HA2 | 18       | 0.1           |
| (3,34) | 1:452:A:VAL:HG23 | 1:454:A:GLY:HA3 | 18       | 0.1           |
| (1,73) | 1:532:A:TYR:O    | 1:536:A:ILE:H   | 16       | 0.1           |
| (1,73) | 1:532:A:TYR:O    | 1:536:A:ILE:H   | 19       | 0.1           |
| (1,71) | 1:531:A:ARG:O    | 1:535:A:LYS:H   | 8        | 0.1           |
| (1,71) | 1:531:A:ARG:O    | 1:535:A:LYS:H   | 15       | 0.1           |
| (1,71) | 1:531:A:ARG:O    | 1:535:A:LYS:H   | 16       | 0.1           |

## 10 Dihedral-angle violation analysis [i](#)

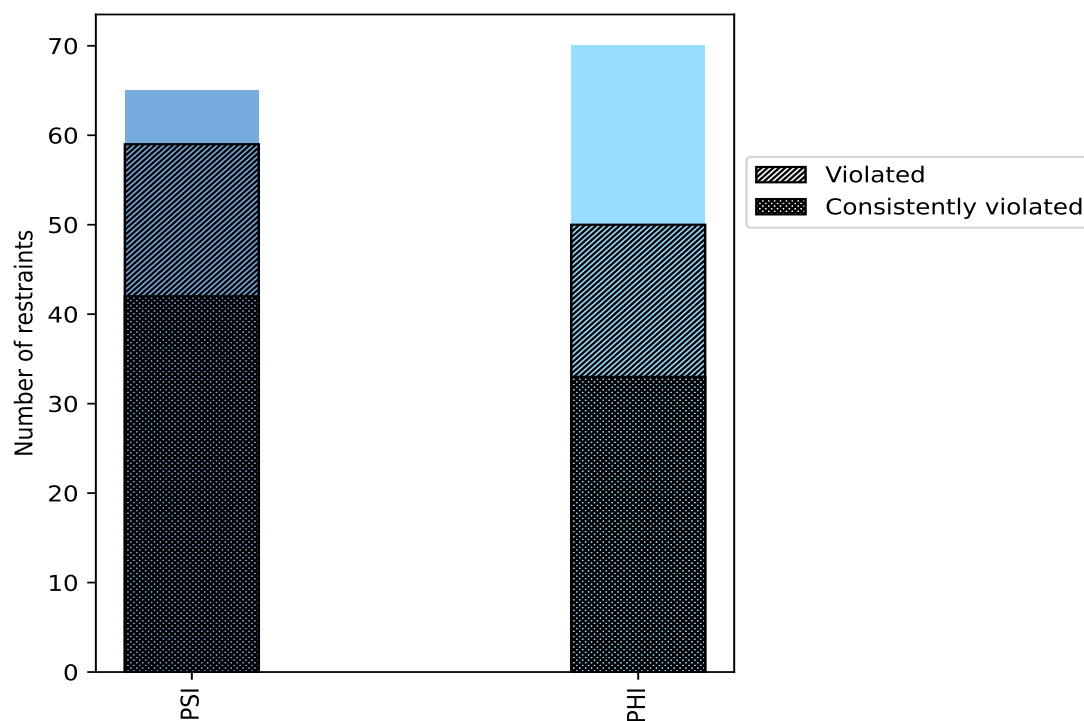
### 10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 65    | 48.1           | 59                    | 90.8           | 43.7           | 42                                 | 64.6           | 31.1           |
| PHI        | 70    | 51.9           | 50                    | 71.4           | 37.0           | 33                                 | 47.1           | 24.4           |
| Total      | 135   | 100.0          | 109                   | 80.7           | 80.7           | 75                                 | 55.6           | 55.6           |

<sup>1</sup> percentage calculated with respect to total number of dihedral-angle restraints, <sup>2</sup> percentage calculated with respect to number of restraints in a particular dihedral-angle type, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

#### 10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



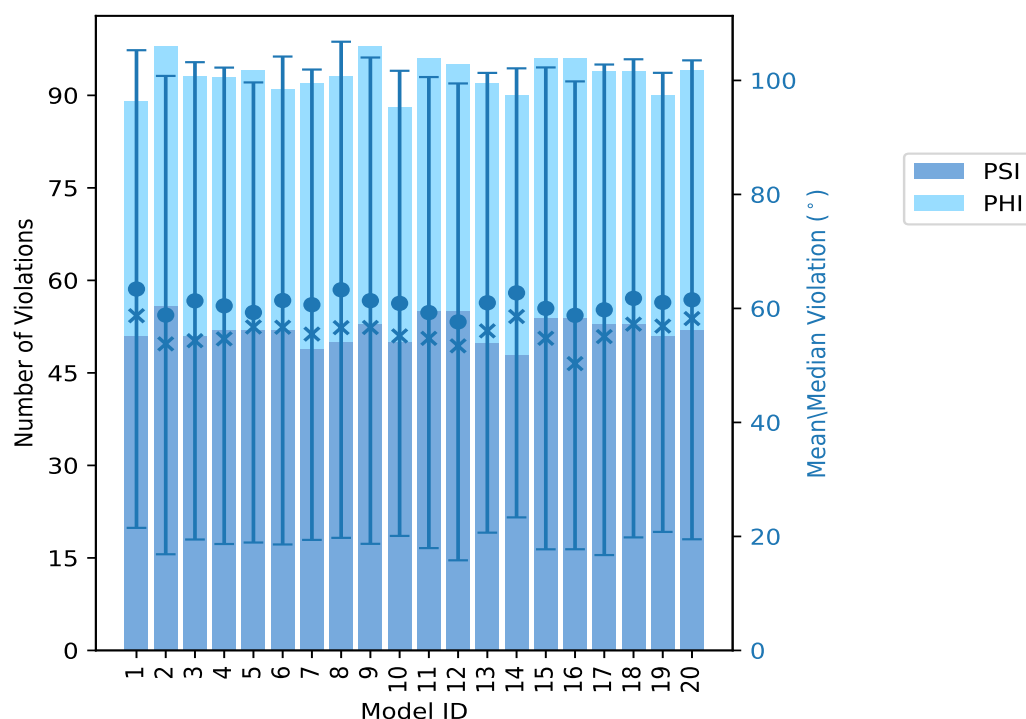
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 51                   | 38  | 89    | 63.4     | 152.53  | 41.9   | 58.72      |
| 2        | 56                   | 42  | 98    | 58.83    | 156.87  | 41.96  | 53.78      |
| 3        | 51                   | 42  | 93    | 61.33    | 155.48  | 41.87  | 54.34      |
| 4        | 52                   | 41  | 93    | 60.46    | 152.68  | 41.79  | 54.66      |
| 5        | 52                   | 42  | 94    | 59.29    | 151.79  | 40.36  | 56.74      |
| 6        | 52                   | 39  | 91    | 61.39    | 155.87  | 42.8   | 56.7       |
| 7        | 49                   | 43  | 92    | 60.65    | 151.16  | 41.26  | 55.5       |
| 8        | 50                   | 43  | 93    | 63.27    | 154.97  | 43.52  | 56.63      |
| 9        | 53                   | 45  | 98    | 61.36    | 170.14  | 42.66  | 56.66      |
| 10       | 50                   | 38  | 88    | 60.89    | 152.22  | 40.8   | 55.18      |
| 11       | 55                   | 41  | 96    | 59.27    | 152.79  | 41.32  | 54.75      |
| 12       | 55                   | 40  | 95    | 57.64    | 156.94  | 41.83  | 53.43      |
| 13       | 50                   | 42  | 92    | 60.99    | 152.71  | 40.33  | 56.06      |
| 14       | 48                   | 42  | 90    | 62.73    | 151.3   | 39.39  | 58.58      |
| 15       | 54                   | 42  | 96    | 60.01    | 152.34  | 42.27  | 54.76      |
| 16       | 54                   | 42  | 96    | 58.79    | 152.62  | 41.04  | 50.32      |
| 17       | 53                   | 41  | 94    | 59.76    | 152.12  | 43.03  | 55.06      |
| 18       | 53                   | 41  | 94    | 61.77    | 153.03  | 41.94  | 57.24      |
| 19       | 51                   | 39  | 90    | 61.06    | 152.91  | 40.27  | 56.9       |
| 20       | 52                   | 42  | 94    | 61.51    | 157.18  | 42.01  | 58.22      |

### 10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



The mean(dot), median(x) and the standard deviation are shown in blue with respect to the y axis on the right

### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %    |
| 1                             | 2   | 3     | 1                        | 5.0  |
| 0                             | 2   | 2     | 2                        | 10.0 |
| 0                             | 1   | 1     | 3                        | 15.0 |
| 1                             | 0   | 1     | 4                        | 20.0 |
| 0                             | 0   | 0     | 5                        | 25.0 |
| 0                             | 1   | 1     | 6                        | 30.0 |
| 0                             | 0   | 0     | 7                        | 35.0 |
| 1                             | 0   | 1     | 8                        | 40.0 |
| 1                             | 2   | 3     | 9                        | 45.0 |
| 0                             | 3   | 3     | 10                       | 50.0 |
| 5                             | 0   | 5     | 11                       | 55.0 |

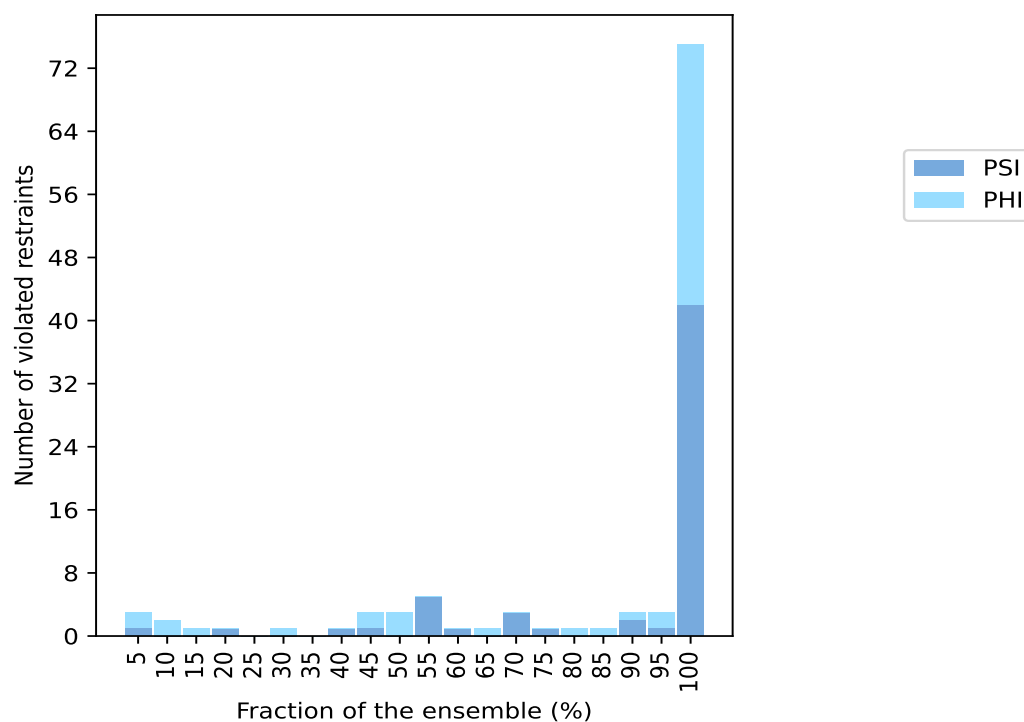
*Continued on next page...*

*Continued from previous page...*

| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 1                             | 0   | 1     | 12                       | 60.0  |
| 0                             | 1   | 1     | 13                       | 65.0  |
| 3                             | 0   | 3     | 14                       | 70.0  |
| 1                             | 0   | 1     | 15                       | 75.0  |
| 0                             | 1   | 1     | 16                       | 80.0  |
| 0                             | 1   | 1     | 17                       | 85.0  |
| 2                             | 1   | 3     | 18                       | 90.0  |
| 1                             | 2   | 3     | 19                       | 95.0  |
| 42                            | 33  | 75    | 20                       | 100.0 |

<sup>1</sup> Number of models with violations

### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

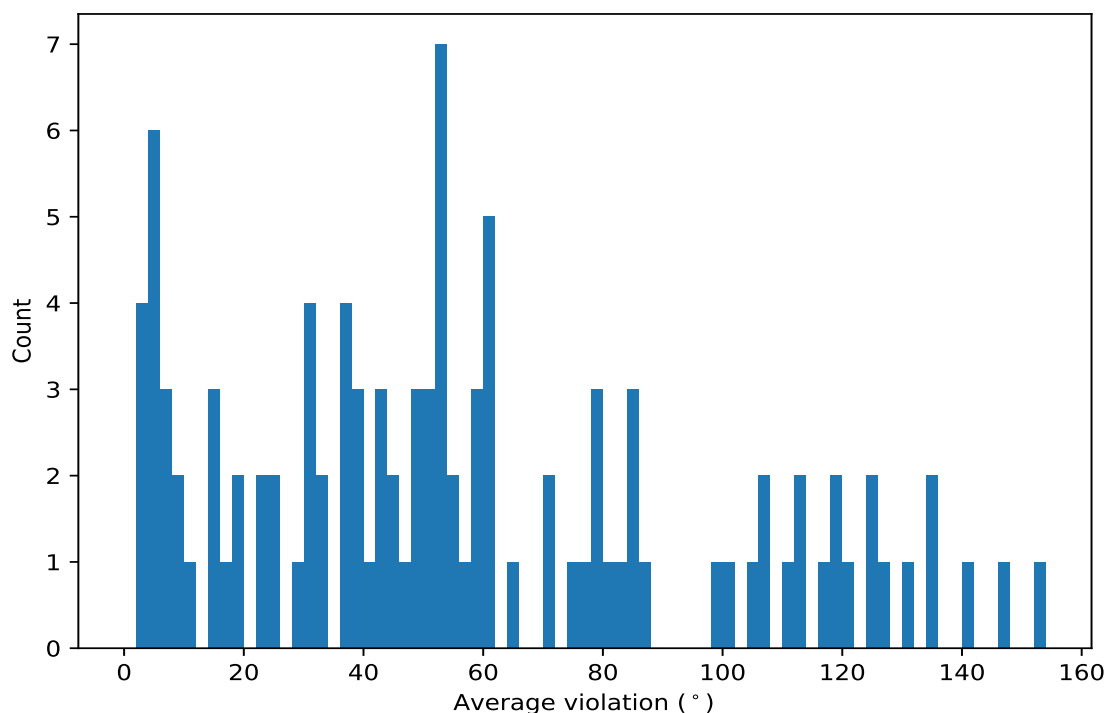


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle restraints ⓘ

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean   | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|--------|-----------------|--------|
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 20                  | 152.22 | 0.54            | 152.28 |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 20                  | 146.26 | 12.48           | 150.7  |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 20                  | 140.07 | 4.28            | 140.23 |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 20                  | 134.86 | 2.43            | 135.2  |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 20                  | 134.65 | 3.57            | 135.68 |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 20                  | 131.88 | 2.18            | 131.9  |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 20                  | 127.07 | 5.56            | 128.13 |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 20                  | 125.05 | 3.72            | 125.9  |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 20                  | 124.65 | 4.12            | 126.32 |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 20                  | 121.13 | 5.98            | 122.48 |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C  | 1:460:A:ILE:N | 20                  | 119.03 | 2.08            | 118.97 |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 20                  | 118.97 | 7.5             | 117.45 |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 20                  | 116.5  | 4.52            | 115.83 |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 20                  | 113.71 | 2.94            | 113.76 |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 20                  | 113.32 | 8.88            | 113.88 |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 20                  | 111.32 | 6.76            | 111.28 |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 20                  | 107.12 | 16.24           | 119.74 |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 20                  | 104.59 | 7.83            | 105.11 |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 20                  | 100.8  | 32.08           | 114.65 |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 20                  | 98.8   | 5.06            | 98.74  |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 20                  | 87.42 | 7.76            | 89.62  |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 20                  | 85.37 | 21.05           | 75.12  |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 20                  | 85.15 | 9.15            | 84.79  |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 20                  | 82.65 | 54.51           | 72.09  |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 20                  | 80.13 | 11.65           | 87.71  |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 20                  | 79.41 | 0.52            | 79.5   |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 20                  | 78.75 | 1.89            | 78.04  |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 20                  | 78.28 | 12.79           | 82.16  |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 20                  | 76.4  | 4.8             | 74.82  |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 20                  | 74.2  | 3.27            | 74.26  |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 20                  | 70.84 | 9.1             | 76.75  |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 20                  | 70.55 | 5.76            | 69.96  |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 20                  | 64.27 | 0.41            | 64.26  |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 20                  | 61.94 | 2.03            | 62.57  |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 20                  | 60.58 | 0.86            | 60.82  |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 20                  | 60.43 | 3.43            | 61.0   |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 20                  | 60.26 | 4.76            | 59.86  |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 20                  | 59.45 | 2.71            | 59.86  |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 20                  | 59.36 | 1.99            | 59.76  |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 20                  | 58.88 | 0.43            | 58.8   |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 20                  | 57.15 | 0.39            | 57.11  |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 20                  | 54.85 | 12.53           | 55.14  |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 20                  | 53.7  | 5.9             | 55.44  |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 20                  | 52.62 | 15.91           | 53.39  |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 20                  | 52.53 | 0.6             | 52.49  |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 20                  | 51.05 | 0.49            | 51.1   |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 20                  | 50.89 | 3.22            | 50.5   |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 20                  | 49.55 | 11.98           | 54.05  |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 20                  | 49.35 | 1.78            | 49.71  |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 20                  | 48.6  | 0.34            | 48.72  |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 20                  | 45.33 | 1.87            | 45.05  |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 20                  | 42.69 | 5.47            | 43.18  |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 20                  | 41.05 | 9.24            | 39.11  |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 20                  | 38.01 | 11.8            | 32.76  |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 20                  | 36.02 | 5.05            | 36.58  |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 20                  | 32.9  | 7.22            | 32.86  |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 20                  | 31.88 | 0.77            | 32.09  |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 20                  | 31.71 | 14.65           | 27.13  |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 20                  | 31.71 | 1.84            | 31.82  |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 20                  | 30.64 | 7.83            | 31.15  |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 20                  | 28.07 | 4.67            | 28.33  |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 20                  | 24.28 | 3.2             | 23.16  |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 20                  | 23.89 | 4.53            | 22.38  |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 20                  | 22.33 | 6.18            | 22.34  |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 20                  | 18.9  | 3.75            | 18.87  |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 20                  | 18.11 | 1.9             | 18.24  |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 20                  | 17.65 | 7.61            | 16.92  |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 20                  | 15.45 | 6.33            | 14.6   |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 20                  | 14.93 | 0.78            | 15.0   |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 20                  | 10.71 | 1.6             | 10.8   |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 20                  | 8.91  | 0.43            | 9.0    |

Continued on next page...

Continued from previous page...

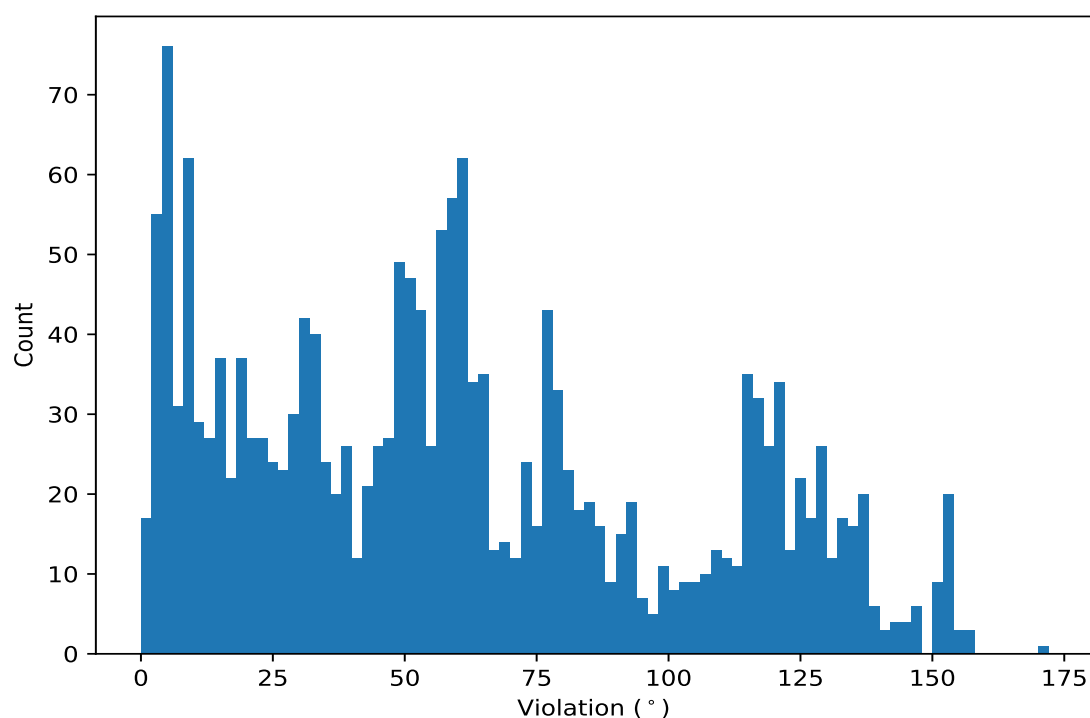
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean   | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|--------|-----------------|--------|
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 20                  | 8.61   | 1.86            | 9.17   |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 20                  | 4.66   | 0.51            | 4.6    |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 20                  | 4.29   | 0.48            | 4.39   |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 20                  | 2.12   | 0.48            | 2.05   |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 19                  | 107.85 | 29.8            | 114.11 |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 19                  | 51.39  | 27.0            | 43.68  |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 19                  | 5.79   | 1.86            | 5.6    |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 18                  | 14.08  | 4.92            | 15.61  |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 18                  | 7.22   | 2.82            | 8.59   |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 18                  | 5.43   | 0.47            | 5.24   |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 17                  | 52.63  | 5.59            | 51.83  |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 16                  | 60.91  | 19.2            | 61.26  |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 15                  | 84.45  | 4.78            | 85.01  |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 14                  | 55.61  | 23.84           | 50.56  |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 14                  | 43.58  | 27.89           | 36.43  |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 14                  | 3.53   | 0.83            | 3.8    |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 13                  | 46.86  | 20.99           | 48.61  |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 12                  | 52.69  | 25.54           | 58.26  |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 11                  | 53.91  | 35.65           | 42.5   |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 11                  | 53.86  | 24.38           | 62.33  |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 11                  | 42.61  | 33.58           | 26.39  |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 11                  | 25.02  | 30.45           | 10.1   |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 11                  | 2.63   | 0.44            | 2.75   |
| (1,3)   | 1:438:A:HIS:C | 1:439:A:HIS:N  | 1:439:A:HIS:CA | 1:439:A:HIS:C | 10                  | 39.78  | 22.65           | 43.4   |
| (1,12)  | 1:444:A:SER:C | 1:445:A:ASN:N  | 1:445:A:ASN:CA | 1:445:A:ASN:C | 10                  | 37.69  | 23.68           | 29.56  |
| (1,11)  | 1:443:A:HIS:C | 1:444:A:SER:N  | 1:444:A:SER:CA | 1:444:A:SER:C | 10                  | 32.89  | 19.19           | 39.61  |
| (1,9)   | 1:442:A:HIS:C | 1:443:A:HIS:N  | 1:443:A:HIS:CA | 1:443:A:HIS:C | 9                   | 45.81  | 22.74           | 45.31  |
| (1,16)  | 1:446:A:ALA:C | 1:447:A:THR:N  | 1:447:A:THR:CA | 1:447:A:THR:C | 9                   | 37.6   | 13.87           | 43.47  |
| (1,108) | 1:516:A:LYS:N | 1:516:A:LYS:CA | 1:516:A:LYS:C  | 1:517:A:HIS:N | 9                   | 7.41   | 3.6             | 8.45   |
| (1,51)  | 1:479:A:SER:N | 1:479:A:SER:CA | 1:479:A:SER:C  | 1:480:A:GLU:N | 8                   | 5.14   | 2.94            | 5.09   |
| (1,111) | 1:517:A:HIS:C | 1:518:A:CYS:N  | 1:518:A:CYS:CA | 1:518:A:CYS:C | 6                   | 5.14   | 2.2             | 4.84   |
| (1,29)  | 1:462:A:THR:N | 1:462:A:THR:CA | 1:462:A:THR:C  | 1:463:A:GLU:N | 4                   | 7.63   | 3.02            | 7.38   |
| (1,63)  | 1:487:A:LEU:C | 1:488:A:GLU:N  | 1:488:A:GLU:CA | 1:488:A:GLU:C | 3                   | 39.04  | 5.56            | 39.43  |
| (1,34)  | 1:464:A:PRO:C | 1:465:A:LEU:N  | 1:465:A:LEU:CA | 1:465:A:LEU:C | 2                   | 36.0   | 19.52           | 36.0   |
| (1,105) | 1:514:A:ASN:C | 1:515:A:LYS:N  | 1:515:A:LYS:CA | 1:515:A:LYS:C | 2                   | 3.95   | 0.99            | 3.95   |

<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



### 10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 9        | 170.14        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 20       | 157.18        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 12       | 156.94        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 2        | 156.87        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 6        | 155.87        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 3        | 155.48        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 8        | 154.97        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 6        | 153.04        |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 18       | 153.03        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 19       | 152.91        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 20       | 152.91        |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 8        | 152.81        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 11       | 152.79        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 13       | 152.71        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 4        | 152.68        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 3        | 152.66        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 16       | 152.62        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 1        | 152.53        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 2        | 152.46        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 6        | 152.46        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 13       | 152.37        |

*Continued on next page...*

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 15       | 152.34        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 10       | 152.22        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 4        | 152.18        |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 20       | 152.15        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 17       | 152.12        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 8        | 152.07        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 9        | 151.81        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 15       | 151.81        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 5        | 151.79        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 12       | 151.61        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 18       | 151.51        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 16       | 151.37        |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 14       | 151.3         |
| (1,123) | 1:525:A:SER:N | 1:525:A:SER:CA | 1:525:A:SER:C  | 1:526:A:GLY:N | 7        | 151.16        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 1        | 150.04        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 17       | 147.84        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 9        | 147.6         |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 18       | 147.09        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 9        | 146.16        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 14       | 146.13        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 4        | 146.11        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 7        | 145.83        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 1        | 145.82        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 2        | 145.18        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 11       | 145.16        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 8        | 143.55        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 11       | 142.86        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 19       | 142.28        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 10       | 142.27        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 17       | 141.04        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 14       | 140.28        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 13       | 140.18        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 7        | 139.99        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 11       | 139.75        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 3        | 138.9         |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 9        | 138.73        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 6        | 138.64        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 5        | 138.21        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 13       | 137.95        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 4        | 137.77        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 4        | 137.65        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 11       | 137.55        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 3        | 137.48        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 5        | 137.39        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 7        | 137.11        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 12       | 136.83        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 6        | 136.81        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 16       | 136.69        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 8        | 136.69        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 5        | 136.6         |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 2        | 136.57        |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 16       | 136.52        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 17       | 136.44        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 2        | 136.42        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 15       | 136.36        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 15       | 136.07        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 19       | 136.03        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 20       | 136.01        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 8        | 135.52        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 3        | 135.34        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 15       | 135.24        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 6        | 135.23        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 20       | 135.18        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 9        | 135.1         |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 10       | 135.04        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 20       | 134.91        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 10       | 134.81        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 7        | 134.68        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 10       | 134.54        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 14       | 134.41        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 12       | 134.34        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 12       | 134.13        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 13       | 134.12        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 16       | 134.03        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 9        | 133.89        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 18       | 133.81        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 12       | 133.8         |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 17       | 133.75        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 17       | 133.59        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 10       | 133.25        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 6        | 133.23        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 17       | 133.16        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 11       | 133.13        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 16       | 132.8         |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 8        | 132.77        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 2        | 132.65        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 19       | 132.59        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 7        | 132.38        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 18       | 132.27        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 14       | 132.12        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 2        | 132.02        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 7        | 131.86        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 1        | 131.75        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 19       | 131.7         |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 1        | 131.7         |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 17       | 131.68        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 20       | 131.43        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 15       | 131.27        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 6        | 131.21        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 4        | 131.14        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 1        | 131.11        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 7        | 130.97        |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 12       | 130.16        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 18       | 129.68        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 14       | 129.57        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 8        | 129.52        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 1        | 129.42        |
| (1,82)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:LYS:N | 18       | 129.4         |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 11       | 129.39        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 3        | 129.3         |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 15       | 129.1         |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 12       | 129.09        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 16       | 128.91        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 13       | 128.89        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 10       | 128.85        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 11       | 128.84        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 5        | 128.76        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 20       | 128.76        |
| (1,74)  | 1:493:A:CYS:N | 1:493:A:CYS:CA | 1:493:A:CYS:C  | 1:494:A:HIS:N | 5        | 128.71        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 3        | 128.68        |
| (1,113) | 1:519:A:TRP:N | 1:519:A:TRP:CA | 1:519:A:TRP:C  | 1:520:A:LYS:N | 7        | 128.59        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 18       | 128.58        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 13       | 128.57        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 11       | 128.52        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 3        | 128.48        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 9        | 128.36        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 13       | 128.25        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 19       | 128.2         |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 15       | 128.11        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 17       | 127.89        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 17       | 127.84        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 8        | 127.75        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 9        | 127.58        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 9        | 127.55        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 18       | 127.38        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 16       | 127.33        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 15       | 127.28        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 4        | 127.21        |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 2        | 127.21        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 10       | 127.16        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 6        | 126.99        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 6        | 126.93        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 19       | 126.69        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 8        | 126.43        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 14       | 126.19        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 3        | 126.14        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 1        | 125.94        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 10       | 125.92        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 18       | 125.87        |
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 1        | 125.77        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 9        | 125.54        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 8        | 125.44        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 4        | 125.36        |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,30)  | 1:462:A:THR:C | 1:463:A:GLU:N  | 1:463:A:GLU:CA | 1:463:A:GLU:C | 19       | 125.26        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 5        | 125.08        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 12       | 125.02        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 7        | 124.86        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 5        | 124.85        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 4        | 124.85        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 4        | 124.64        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 12       | 124.57        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 20       | 124.57        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 9        | 124.52        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 1        | 124.41        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 20       | 124.37        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 19       | 124.2         |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 7        | 124.12        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 11       | 124.02        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 8        | 123.99        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 2        | 123.97        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C  | 1:460:A:ILE:N | 6        | 123.95        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 7        | 123.73        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 16       | 123.56        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 2        | 123.4         |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 17       | 123.29        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 13       | 123.19        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C  | 1:460:A:ILE:N | 7        | 123.16        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 15       | 123.01        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 16       | 122.5         |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 19       | 122.45        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 16       | 122.23        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 13       | 121.99        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 12       | 121.89        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 15       | 121.85        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 11       | 121.8         |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 12       | 121.64        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 14       | 121.61        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 1        | 121.42        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 9        | 121.41        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 15       | 121.28        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C  | 1:460:A:ILE:N | 2        | 121.28        |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 3        | 121.03        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 1        | 120.97        |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 11       | 120.95        |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 15       | 120.92        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 16       | 120.9         |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 10       | 120.88        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 5        | 120.76        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 7        | 120.76        |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 17       | 120.71        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 14       | 120.64        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 4        | 120.63        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 20       | 120.62        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 19       | 120.55        |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C | 1:457:A:VAL:N | 2        | 120.5         |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 19       | 120.46        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C | 1:497:A:PHE:N | 4        | 120.42        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C | 1:518:A:CYS:N | 18       | 120.36        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C | 1:527:A:ASP:N | 18       | 120.31        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C | 1:493:A:CYS:N | 16       | 120.3         |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 14       | 120.27        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C | 1:497:A:PHE:N | 1        | 120.26        |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C | 1:457:A:VAL:N | 9        | 120.23        |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C | 1:457:A:VAL:N | 19       | 120.14        |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C | 1:457:A:VAL:N | 1        | 120.01        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C | 1:497:A:PHE:N | 7        | 119.87        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C | 1:522:A:GLU:N | 1        | 119.82        |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C | 1:457:A:VAL:N | 20       | 119.8         |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C | 1:457:A:VAL:N | 4        | 119.69        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C | 1:497:A:PHE:N | 14       | 119.51        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 8        | 119.5         |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 17       | 119.43        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C | 1:527:A:ASP:N | 11       | 119.38        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 1        | 119.3         |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 10       | 119.28        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C | 1:489:A:GLY:N | 16       | 119.16        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 20       | 119.1         |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C | 1:457:A:VAL:N | 8        | 118.85        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 3        | 118.84        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 12       | 118.79        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C | 1:522:A:GLU:N | 20       | 118.7         |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C | 1:523:A:ILE:N | 5        | 118.65        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 4        | 118.53        |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C | 1:442:A:HIS:N | 1        | 118.42        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C | 1:522:A:GLU:N | 9        | 118.41        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C | 1:489:A:GLY:N | 6        | 118.35        |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C | 1:442:A:HIS:N | 15       | 118.29        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C | 1:493:A:CYS:N | 4        | 118.23        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C | 1:489:A:GLY:N | 17       | 118.19        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C | 1:497:A:PHE:N | 9        | 118.18        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 11       | 118.08        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 18       | 117.95        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C | 1:497:A:PHE:N | 2        | 117.92        |
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C | 1:491:A:THR:N | 5        | 117.86        |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C | 1:442:A:HIS:N | 3        | 117.82        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C | 1:459:A:ILE:N | 7        | 117.78        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C | 1:518:A:CYS:N | 2        | 117.68        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C | 1:459:A:ILE:N | 5        | 117.62        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C | 1:459:A:ILE:N | 14       | 117.44        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C | 1:459:A:ILE:N | 6        | 117.41        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C | 1:527:A:ASP:N | 8        | 117.39        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1:460:A:ILE:N | 15       | 117.31        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C | 1:527:A:ASP:N | 20       | 117.28        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C | 1:522:A:GLU:N | 2        | 117.2         |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C | 1:489:A:GLY:N | 4        | 117.11        |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,68)  | 1:490:A:ASP:N | 1:490:A:ASP:CA | 1:490:A:ASP:C  | 1:491:A:THR:N | 10       | 117.09        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C  | 1:460:A:ILE:N | 13       | 117.08        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 13       | 117.08        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C  | 1:460:A:ILE:N | 9        | 117.02        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 3        | 117.01        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 3        | 117.0         |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 4        | 116.95        |
| (1,115) | 1:520:A:LYS:N | 1:520:A:LYS:CA | 1:520:A:LYS:C  | 1:521:A:LEU:N | 14       | 116.88        |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 5        | 116.88        |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 19       | 116.86        |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 10       | 116.82        |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 8        | 116.8         |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 14       | 116.67        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 18       | 116.6         |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 2        | 116.57        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 3        | 116.42        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 18       | 116.38        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 17       | 116.09        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C  | 1:460:A:ILE:N | 5        | 115.99        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 10       | 115.86        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 19       | 115.8         |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 5        | 115.77        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 12       | 115.77        |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 17       | 115.75        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 19       | 115.74        |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 3        | 115.55        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 6        | 115.47        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 12       | 115.45        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 20       | 115.45        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 17       | 115.38        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 14       | 115.37        |
| (1,25)  | 1:459:A:ILE:N | 1:459:A:ILE:CA | 1:459:A:ILE:C  | 1:460:A:ILE:N | 16       | 115.35        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 9        | 115.32        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 7        | 115.25        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 3        | 115.25        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 18       | 115.22        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 8        | 115.18        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 11       | 115.05        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 16       | 115.03        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 15       | 114.9         |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 14       | 114.88        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 8        | 114.87        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 15       | 114.85        |
| (1,78)  | 1:495:A:ALA:N | 1:495:A:ALA:CA | 1:495:A:ALA:C  | 1:496:A:ARG:N | 8        | 114.79        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 5        | 114.76        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 11       | 114.74        |
| (1,119) | 1:522:A:GLU:N | 1:522:A:GLU:CA | 1:522:A:GLU:C  | 1:523:A:ILE:N | 13       | 114.56        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 20       | 114.42        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 20       | 114.24        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 15       | 114.24        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 12       | 114.11        |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 11       | 114.05        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 2        | 114.01        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 10       | 113.51        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 18       | 113.42        |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 20       | 113.18        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 19       | 113.15        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 13       | 113.11        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 8        | 112.52        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 4        | 112.5         |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 1        | 112.35        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 20       | 112.16        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 1        | 112.05        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 6        | 112.03        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 1        | 111.7         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 10       | 111.51        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 10       | 111.32        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 6        | 111.3         |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 6        | 111.25        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 3        | 111.17        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 3        | 111.07        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 17       | 110.99        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 9        | 110.64        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 13       | 110.43        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 3        | 110.15        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 4        | 110.13        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 5        | 109.7         |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 12       | 109.58        |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 3        | 109.47        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 15       | 109.17        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 17       | 109.14        |
| (1,23)  | 1:458:A:LYS:N | 1:458:A:LYS:CA | 1:458:A:LYS:C  | 1:459:A:ILE:N | 8        | 109.11        |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 9        | 109.02        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 15       | 108.97        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 13       | 108.93        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 10       | 108.88        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 14       | 108.88        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 19       | 108.6         |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 16       | 108.56        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 10       | 107.76        |
| (1,72)  | 1:492:A:GLU:N | 1:492:A:GLU:CA | 1:492:A:GLU:C  | 1:493:A:CYS:N | 5        | 107.62        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 18       | 107.58        |
| (1,80)  | 1:496:A:ARG:N | 1:496:A:ARG:CA | 1:496:A:ARG:C  | 1:497:A:PHE:N | 6        | 107.43        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 16       | 107.09        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 14       | 106.78        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 9        | 106.71        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 15       | 106.37        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 2        | 106.14        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 6        | 106.05        |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 8        | 105.96        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 4        | 105.93        |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 9        | 105.75        |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 10       | 105.4         |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 18       | 105.27        |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 6        | 105.23        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 7        | 104.95        |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 11       | 104.76        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 11       | 104.44        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 1        | 103.98        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 12       | 103.73        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 16       | 103.69        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 7        | 103.65        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 13       | 103.29        |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 17       | 103.23        |
| (1,110) | 1:517:A:HIS:N | 1:517:A:HIS:CA | 1:517:A:HIS:C  | 1:518:A:CYS:N | 20       | 103.06        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 19       | 102.56        |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 13       | 102.03        |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 15       | 101.99        |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 11       | 101.79        |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 4        | 101.39        |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 11       | 101.03        |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 8        | 100.88        |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 13       | 100.83        |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 5        | 100.83        |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 14       | 100.51        |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 8        | 99.68         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 18       | 99.28         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 12       | 99.02         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 14       | 98.94         |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 13       | 98.88         |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 18       | 98.73         |
| (1,117) | 1:521:A:LEU:N | 1:521:A:LEU:CA | 1:521:A:LEU:C  | 1:522:A:GLU:N | 12       | 98.64         |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 2        | 98.55         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 19       | 98.55         |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 20       | 98.46         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 13       | 98.29         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 6        | 97.42         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 2        | 96.83         |
| (1,125) | 1:526:A:GLY:N | 1:526:A:GLY:CA | 1:526:A:GLY:C  | 1:527:A:ASP:N | 17       | 96.69         |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 18       | 96.15         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 5        | 96.13         |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 17       | 95.88         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 1        | 95.15         |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 2        | 95.09         |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 18       | 94.99         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 16       | 94.82         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 4        | 94.75         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 20       | 94.64         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 12       | 93.96         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 6        | 93.89         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 6        | 93.77         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 19       | 93.68         |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 2        | 93.67         |

Continued on next page...

*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 9        | 93.51         |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 17       | 93.2          |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 18       | 93.12         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 1        | 93.06         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 5        | 92.8          |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 1        | 92.71         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 14       | 92.71         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 9        | 92.7          |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 2        | 92.51         |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 19       | 92.49         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 8        | 92.37         |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 8        | 92.25         |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 3        | 92.16         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 6        | 92.09         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 16       | 91.76         |
| (1,21)  | 1:457:A:VAL:N | 1:457:A:VAL:CA | 1:457:A:VAL:C  | 1:458:A:LYS:N | 3        | 91.74         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 10       | 91.67         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 15       | 91.62         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 19       | 91.51         |
| (1,76)  | 1:494:A:HIS:N | 1:494:A:HIS:CA | 1:494:A:HIS:C  | 1:495:A:ALA:N | 7        | 91.24         |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 13       | 91.2          |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 14       | 91.12         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 3        | 90.86         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 13       | 90.78         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 1        | 90.65         |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 5        | 90.56         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 17       | 90.51         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 8        | 90.22         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 17       | 90.1          |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 15       | 89.6          |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 9        | 89.07         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 8        | 88.73         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 8        | 88.39         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 10       | 88.37         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 18       | 88.29         |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 14       | 88.19         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 3        | 88.15         |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 7        | 88.02         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 17       | 87.93         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 13       | 87.78         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 6        | 87.63         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 18       | 87.62         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 7        | 87.49         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 14       | 87.38         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 3        | 87.27         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 4        | 87.26         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 5        | 86.96         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 10       | 86.86         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 19       | 86.7          |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 18       | 86.59         |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 13       | 86.38         |

*Continued on next page...*

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 16       | 86.35         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 4        | 86.26         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 9        | 86.18         |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 12       | 85.98         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 10       | 85.85         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 17       | 85.72         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 13       | 85.68         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 10       | 85.59         |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 15       | 85.05         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 2        | 85.01         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 18       | 84.87         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 3        | 84.74         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 7        | 84.71         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 15       | 84.55         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 18       | 84.52         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 14       | 84.51         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 2        | 84.49         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 5        | 84.47         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 5        | 84.37         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 12       | 84.31         |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 6        | 84.14         |
| (1,20)  | 1:456:A:ILE:N | 1:456:A:ILE:CA | 1:456:A:ILE:C  | 1:457:A:VAL:N | 16       | 84.03         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 16       | 83.81         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 15       | 83.79         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 16       | 83.32         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 11       | 83.26         |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 18       | 83.07         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 14       | 83.05         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 20       | 82.98         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 6        | 82.88         |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 15       | 82.7          |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 4        | 82.54         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 11       | 82.5          |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 20       | 82.49         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 16       | 82.47         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 17       | 82.31         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 11       | 82.24         |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 16       | 82.24         |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 1        | 82.15         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 7        | 82.0          |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 1        | 81.93         |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 14       | 81.86         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 2        | 81.71         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 11       | 81.51         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 16       | 81.42         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 3        | 81.34         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 5        | 81.31         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 19       | 81.29         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 2        | 81.29         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 2        | 81.15         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 15       | 80.82         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 13       | 80.72         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 3        | 80.68         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 6        | 80.65         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 13       | 80.55         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 4        | 80.5          |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 1        | 80.45         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 20       | 80.43         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 11       | 80.41         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 4        | 80.35         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 6        | 80.21         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 9        | 80.11         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 16       | 80.0          |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 17       | 79.98         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 8        | 79.92         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 12       | 79.84         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 10       | 79.64         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 14       | 79.62         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 3        | 79.59         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 16       | 79.56         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 1        | 79.5          |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 5        | 79.49         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 9        | 79.48         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 16       | 79.36         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 11       | 79.26         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 7        | 79.24         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 20       | 79.23         |
| (1,12)  | 1:444:A:SER:C | 1:445:A:ASN:N  | 1:445:A:ASN:CA | 1:445:A:ASN:C | 7        | 79.21         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 18       | 79.2          |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 2        | 79.18         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 3        | 79.16         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 19       | 79.01         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 4        | 78.96         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 1        | 78.95         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 7        | 78.88         |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 7        | 78.83         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 13       | 78.76         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 11       | 78.73         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 15       | 78.54         |
| (1,46)  | 1:475:A:LEU:C | 1:476:A:ALA:N  | 1:476:A:ALA:CA | 1:476:A:ALA:C | 19       | 78.51         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 9        | 78.2          |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 8        | 78.13         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 2        | 78.11         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 14       | 78.02         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 8        | 78.02         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 12       | 78.0          |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 11       | 77.99         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 17       | 77.96         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 10       | 77.93         |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 5        | 77.9          |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 2        | 77.85         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 7        | 77.85         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 4        | 77.84         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 18       | 77.79         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 3        | 77.77         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 5        | 77.76         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 2        | 77.74         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 13       | 77.6          |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 20       | 77.52         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 1        | 77.48         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 14       | 77.4          |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 15       | 77.32         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 12       | 77.2          |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 10       | 77.17         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 15       | 77.11         |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 9        | 77.05         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 12       | 77.04         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 12       | 76.97         |
| (1,9)   | 1:442:A:HIS:C | 1:443:A:HIS:N  | 1:443:A:HIS:CA | 1:443:A:HIS:C | 18       | 76.9          |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 6        | 76.89         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 10       | 76.88         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 6        | 76.85         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 6        | 76.79         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 8        | 76.77         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 8        | 76.76         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 12       | 76.75         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 18       | 76.74         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 15       | 76.74         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 17       | 76.73         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 16       | 76.72         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 5        | 76.71         |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 2        | 76.61         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 15       | 76.58         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 14       | 76.53         |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 16       | 76.47         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 9        | 76.46         |
| (1,18)  | 1:455:A:VAL:N | 1:455:A:VAL:CA | 1:455:A:VAL:C  | 1:456:A:ILE:N | 20       | 76.43         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 18       | 76.3          |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 12       | 76.22         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 17       | 75.54         |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 2        | 75.46         |
| (1,122) | 1:524:A:LEU:C | 1:525:A:SER:N  | 1:525:A:SER:CA | 1:525:A:SER:C | 7        | 75.45         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 12       | 75.2          |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 3        | 75.06         |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 9        | 74.93         |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 5        | 74.8          |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 19       | 74.59         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 20       | 74.57         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 10       | 74.56         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 9        | 74.3          |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 4        | 74.27         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 5        | 74.24         |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 1        | 74.03         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 9        | 74.02         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 2        | 74.0          |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 8        | 73.92         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 6        | 73.87         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 6        | 73.84         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 19       | 73.71         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 17       | 73.51         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 11       | 73.49         |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 11       | 73.45         |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 7        | 73.23         |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 9        | 73.07         |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 18       | 73.05         |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 19       | 72.92         |
| (1,9)   | 1:442:A:HIS:C | 1:443:A:HIS:N  | 1:443:A:HIS:CA | 1:443:A:HIS:C | 13       | 72.84         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 11       | 72.73         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 17       | 72.71         |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 12       | 72.71         |
| (1,3)   | 1:438:A:HIS:C | 1:439:A:HIS:N  | 1:439:A:HIS:CA | 1:439:A:HIS:C | 5        | 72.7          |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 13       | 72.65         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 3        | 72.63         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 20       | 72.49         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 20       | 72.47         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 9        | 72.45         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 1        | 72.41         |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 14       | 72.17         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 13       | 72.04         |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 20       | 71.8          |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 1        | 71.52         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 19       | 71.23         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 4        | 71.0          |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 13       | 70.93         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 8        | 70.9          |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 8        | 70.74         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 14       | 70.71         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 19       | 70.63         |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 10       | 70.23         |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 6        | 70.22         |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 13       | 70.12         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 2        | 69.83         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 19       | 69.67         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 14       | 69.63         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 17       | 69.58         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 20       | 69.4          |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 1        | 69.2          |
| (1,85)  | 1:498:A:LYS:C | 1:499:A:THR:N  | 1:499:A:THR:CA | 1:499:A:THR:C | 1        | 68.95         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 19       | 68.92         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 7        | 68.72         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 7        | 68.71         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 7        | 68.48         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 15       | 68.48         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 14       | 68.33         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 6        | 68.07         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 16       | 67.97         |
| (1,12)  | 1:444:A:SER:C | 1:445:A:ASN:N  | 1:445:A:ASN:CA | 1:445:A:ASN:C | 20       | 67.58         |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 5        | 67.22         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 16       | 67.13         |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 8        | 67.12         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 13       | 67.08         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 4        | 67.04         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 12       | 66.73         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 11       | 66.7          |
| (1,12)  | 1:444:A:SER:C | 1:445:A:ASN:N  | 1:445:A:ASN:CA | 1:445:A:ASN:C | 9        | 66.67         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 7        | 66.42         |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 7        | 66.27         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 14       | 66.06         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 11       | 65.88         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 10       | 65.81         |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 14       | 65.41         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 20       | 65.4          |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 16       | 65.3          |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 17       | 65.27         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 15       | 65.2          |
| (1,109) | 1:516:A:LYS:C | 1:517:A:HIS:N  | 1:517:A:HIS:CA | 1:517:A:HIS:C | 20       | 65.18         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 5        | 65.01         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 20       | 64.94         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 12       | 64.94         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 18       | 64.94         |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 20       | 64.8          |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 3        | 64.76         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 14       | 64.76         |
| (1,116) | 1:520:A:LYS:C | 1:521:A:LEU:N  | 1:521:A:LEU:CA | 1:521:A:LEU:C | 3        | 64.68         |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 4        | 64.68         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 4        | 64.61         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 15       | 64.6          |
| (1,9)   | 1:442:A:HIS:C | 1:443:A:HIS:N  | 1:443:A:HIS:CA | 1:443:A:HIS:C | 2        | 64.52         |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 5        | 64.49         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 16       | 64.43         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 3        | 64.42         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 11       | 64.32         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 19       | 64.31         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 17       | 64.27         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 2        | 64.27         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 5        | 64.26         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 6        | 64.25         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 13       | 64.24         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 7        | 64.19         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 17       | 64.17         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 10       | 64.1          |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 10       | 64.08         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 18       | 64.04         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 8        | 63.95         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 18       | 63.92         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 2        | 63.91         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 16       | 63.89         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 10       | 63.89         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 5        | 63.89         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 7        | 63.86         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 7        | 63.78         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 11       | 63.76         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 7        | 63.76         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 9        | 63.74         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 1        | 63.72         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 1        | 63.71         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 20       | 63.66         |
| (1,26)  | 1:459:A:ILE:C | 1:460:A:ILE:N  | 1:460:A:ILE:CA | 1:460:A:ILE:C | 9        | 63.56         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 12       | 63.54         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 20       | 63.53         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 10       | 63.39         |
| (1,45)  | 1:474:A:THR:N | 1:474:A:THR:CA | 1:474:A:THR:C  | 1:475:A:LEU:N | 2        | 63.25         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 15       | 62.87         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 19       | 62.8          |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 3        | 62.76         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 19       | 62.75         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 13       | 62.73         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 11       | 62.72         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 16       | 62.5          |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 1        | 62.45         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 8        | 62.42         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 9        | 62.42         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 9        | 62.35         |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 19       | 62.33         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 10       | 62.27         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 1        | 62.13         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 11       | 62.08         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 8        | 61.96         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 7        | 61.95         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 13       | 61.83         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 3        | 61.83         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 2        | 61.82         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 6        | 61.81         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 6        | 61.74         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 4        | 61.74         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 14       | 61.72         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 5        | 61.71         |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 12       | 61.71         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 11       | 61.66         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 9        | 61.63         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 15       | 61.53         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 9        | 61.48         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 12       | 61.4          |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 6        | 61.39         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 18       | 61.35         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 18       | 61.31         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 15       | 61.28         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 14       | 61.22         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 17       | 61.21         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 1        | 61.16         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 11       | 61.13         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 14       | 61.11         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 18       | 61.07         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 19       | 61.06         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 11       | 61.06         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 4        | 61.05         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 13       | 61.05         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 5        | 61.02         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 9        | 60.99         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 16       | 60.99         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 15       | 60.97         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 13       | 60.94         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 8        | 60.9          |
| (1,3)   | 1:438:A:HIS:C | 1:439:A:HIS:N  | 1:439:A:HIS:CA | 1:439:A:HIS:C | 17       | 60.88         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 18       | 60.86         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 16       | 60.85         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 4        | 60.84         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 14       | 60.79         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 15       | 60.71         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 6        | 60.67         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 18       | 60.62         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 4        | 60.59         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 10       | 60.57         |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 2        | 60.56         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 12       | 60.54         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 8        | 60.53         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 15       | 60.52         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 2        | 60.47         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 12       | 60.45         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 1        | 60.42         |
| (1,11)  | 1:443:A:HIS:C | 1:444:A:SER:N  | 1:444:A:SER:CA | 1:444:A:SER:C | 12       | 60.4          |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 6        | 60.27         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 2        | 60.26         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 17       | 60.21         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 4        | 60.16         |
| (1,65)  | 1:488:A:GLU:C | 1:489:A:GLY:N  | 1:489:A:GLY:CA | 1:489:A:GLY:C | 5        | 60.06         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 8        | 60.03         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 20       | 60.02         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 5        | 60.01         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 16       | 59.98         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 20       | 59.96         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 20       | 59.89         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 5        | 59.82         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 8        | 59.61         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 4        | 59.55         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 20       | 59.51         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 11       | 59.49         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 9        | 59.49         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 9        | 59.47         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 12       | 59.42         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 19       | 59.27         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 16       | 59.23         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 15       | 59.2          |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 1        | 59.19         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 4        | 59.18         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 19       | 59.18         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 7        | 59.18         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 18       | 59.13         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 1        | 59.13         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 5        | 59.12         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 7        | 59.12         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 14       | 59.09         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 4        | 59.08         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 13       | 59.03         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 9        | 59.02         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 19       | 59.02         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 10       | 58.96         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 11       | 58.94         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 19       | 58.92         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 10       | 58.92         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 17       | 58.81         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 3        | 58.78         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 2        | 58.76         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 15       | 58.75         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 11       | 58.75         |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 3        | 58.75         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 1        | 58.72         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 10       | 58.72         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 14       | 58.72         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 13       | 58.7          |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 16       | 58.68         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 18       | 58.64         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 6        | 58.63         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 14       | 58.59         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 2        | 58.58         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 14       | 58.58         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 20       | 58.57         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 16       | 58.56         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 14       | 58.55         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 12       | 58.54         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 20       | 58.52         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 3        | 58.48         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 17       | 58.47         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 13       | 58.4          |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 5        | 58.31         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 17       | 58.05         |
| (1,35)  | 1:465:A:LEU:N | 1:465:A:LEU:CA | 1:465:A:LEU:C  | 1:466:A:PRO:N | 20       | 57.92         |
| (1,97)  | 1:508:A:ASN:N | 1:508:A:ASN:CA | 1:508:A:ASN:C  | 1:509:A:ALA:N | 7        | 57.88         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 13       | 57.88         |
| (1,3)   | 1:438:A:HIS:C | 1:439:A:HIS:N  | 1:439:A:HIS:CA | 1:439:A:HIS:C | 11       | 57.84         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 2        | 57.82         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 1        | 57.78         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 11       | 57.73         |
| (1,39)  | 1:471:A:VAL:N | 1:471:A:VAL:CA | 1:471:A:VAL:C  | 1:472:A:ARG:N | 7        | 57.73         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 15       | 57.69         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 1        | 57.65         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 9        | 57.65         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 18       | 57.64         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 12       | 57.63         |
| (1,91)  | 1:504:A:GLN:N | 1:504:A:GLN:CA | 1:504:A:GLN:C  | 1:505:A:ALA:N | 5        | 57.6          |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 19       | 57.59         |
| (1,3)   | 1:438:A:HIS:C | 1:439:A:HIS:N  | 1:439:A:HIS:CA | 1:439:A:HIS:C | 10       | 57.55         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 4        | 57.53         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 6        | 57.46         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 12       | 57.44         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 3        | 57.41         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 7        | 57.38         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 13       | 57.29         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 5        | 57.25         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 10       | 57.25         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 16       | 57.23         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 19       | 57.12         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 20       | 57.1          |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 8        | 57.08         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 3        | 57.07         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 14       | 57.07         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 12       | 56.99         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 6        | 56.94         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 3        | 56.88         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 18       | 56.85         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 11       | 56.78         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 2        | 56.77         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 9        | 56.76         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 12       | 56.76         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 17       | 56.72         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 6        | 56.7          |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 19       | 56.69         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 8        | 56.63         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 11       | 56.57         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 9        | 56.56         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 4        | 56.54         |
| (1,37)  | 1:470:A:GLN:N | 1:470:A:GLN:CA | 1:470:A:GLN:C  | 1:471:A:VAL:N | 17       | 56.45         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 18       | 56.32         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 5        | 56.24         |
| (1,61)  | 1:485:A:ASP:N | 1:485:A:ASP:CA | 1:485:A:ASP:C  | 1:486:A:LEU:N | 4        | 56.22         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 6        | 56.21         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 4        | 56.08         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 6        | 56.07         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 17       | 56.02         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 15       | 55.96         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 14       | 55.7          |
| (1,34)  | 1:464:A:PRO:C | 1:465:A:LEU:N  | 1:465:A:LEU:CA | 1:465:A:LEU:C | 20       | 55.52         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 10       | 55.47         |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 12       | 55.32         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 1        | 55.09         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 10       | 54.88         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 15       | 54.82         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 13       | 54.82         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 15       | 54.7          |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 4        | 54.66         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 8        | 54.65         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 3        | 54.64         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 14       | 54.62         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 5        | 54.47         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 20       | 54.45         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 15       | 54.43         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 3        | 54.34         |
| (1,41)  | 1:472:A:ARG:N | 1:472:A:ARG:CA | 1:472:A:ARG:C  | 1:473:A:ASP:N | 2        | 54.33         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 10       | 54.28         |
| (1,71)  | 1:491:A:THR:C | 1:492:A:GLU:N  | 1:492:A:GLU:CA | 1:492:A:GLU:C | 8        | 54.24         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 13       | 54.23         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 5        | 54.21         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 17       | 54.11         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 13       | 54.1          |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 18       | 54.0          |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 18       | 53.91         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 4        | 53.8          |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 18       | 53.74         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 4        | 53.63         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 7        | 53.62         |
| (1,75)  | 1:493:A:CYS:C | 1:494:A:HIS:N  | 1:494:A:HIS:CA | 1:494:A:HIS:C | 7        | 53.45         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 12       | 53.43         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 17       | 53.42         |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 19       | 53.36         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 9        | 53.3          |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 1        | 53.28         |
| (1,11)  | 1:443:A:HIS:C | 1:444:A:SER:N  | 1:444:A:SER:CA | 1:444:A:SER:C | 2        | 53.23         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 18       | 53.15         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 8        | 53.14         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 18       | 53.0          |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 6        | 52.97         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 11       | 52.93         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 15       | 52.92         |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 13       | 52.88         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 11       | 52.88         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 18       | 52.74         |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 3        | 52.74         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 3        | 52.72         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 10       | 52.7          |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 14       | 52.64         |

Continued on next page...

*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 2        | 52.62         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 5        | 52.51         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 4        | 52.48         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 19       | 52.47         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 11       | 52.46         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 1        | 52.45         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 6        | 52.45         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 2        | 52.44         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 20       | 52.41         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 11       | 52.35         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 12       | 52.31         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 9        | 52.29         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 12       | 52.27         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 13       | 52.24         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 17       | 52.15         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 7        | 52.13         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 18       | 52.03         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 14       | 52.02         |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 15       | 51.85         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 11       | 51.83         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 7        | 51.83         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 4        | 51.81         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 12       | 51.65         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 2        | 51.63         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 7        | 51.6          |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 2        | 51.58         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 1        | 51.53         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 6        | 51.52         |
| (1,9)   | 1:442:A:HIS:C | 1:443:A:HIS:N  | 1:443:A:HIS:CA | 1:443:A:HIS:C | 4        | 51.45         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 13       | 51.41         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 10       | 51.36         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 6        | 51.33         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 8        | 51.3          |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 11       | 51.25         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 13       | 51.23         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 3        | 51.21         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 18       | 51.19         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 2        | 51.05         |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 14       | 51.03         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 19       | 51.01         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 16       | 50.99         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 20       | 50.97         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 4        | 50.88         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 3        | 50.8          |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 12       | 50.74         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 10       | 50.64         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 17       | 50.62         |
| (1,93)  | 1:505:A:ALA:N | 1:505:A:ALA:CA | 1:505:A:ALA:C  | 1:506:A:VAL:N | 16       | 50.59         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 1        | 50.58         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 1        | 50.5          |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 12       | 50.5          |

*Continued on next page...*

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 5        | 50.48         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 14       | 50.43         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 15       | 50.43         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 20       | 50.39         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 3        | 50.31         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 13       | 50.29         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 5        | 50.26         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 8        | 50.23         |
| (1,24)  | 1:458:A:LYS:C | 1:459:A:ILE:N  | 1:459:A:ILE:CA | 1:459:A:ILE:C | 9        | 50.15         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 5        | 50.12         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 1        | 50.11         |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 18       | 50.1          |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 11       | 50.05         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 16       | 50.04         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 3        | 49.98         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 4        | 49.97         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 19       | 49.94         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 13       | 49.91         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 11       | 49.87         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 9        | 49.85         |
| (1,73)  | 1:492:A:GLU:C | 1:493:A:CYS:N  | 1:493:A:CYS:CA | 1:493:A:CYS:C | 6        | 49.77         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 4        | 49.57         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 9        | 49.5          |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 15       | 49.48         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 2        | 49.28         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 15       | 49.21         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 3        | 49.2          |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 18       | 49.17         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 10       | 49.17         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 8        | 49.11         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 8        | 49.11         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 5        | 49.06         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 7        | 49.04         |
| (1,16)  | 1:446:A:ALA:C | 1:447:A:THR:N  | 1:447:A:THR:CA | 1:447:A:THR:C | 19       | 49.03         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 3        | 48.97         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 5        | 48.92         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 7        | 48.92         |
| (1,118) | 1:521:A:LEU:C | 1:522:A:GLU:N  | 1:522:A:GLU:CA | 1:522:A:GLU:C | 14       | 48.91         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 6        | 48.87         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 14       | 48.84         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 11       | 48.81         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 2        | 48.77         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 10       | 48.75         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 17       | 48.75         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 1        | 48.72         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 20       | 48.72         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 10       | 48.66         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 11       | 48.61         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 4        | 48.59         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 16       | 48.59         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 8        | 48.57         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,16)  | 1:446:A:ALA:C | 1:447:A:THR:N  | 1:447:A:THR:CA | 1:447:A:THR:C | 10       | 48.55         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 9        | 48.53         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 9        | 48.49         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 20       | 48.34         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 13       | 48.33         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 19       | 48.28         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 15       | 48.23         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 20       | 48.2          |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 7        | 48.17         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 16       | 48.08         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 3        | 48.05         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 14       | 48.01         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 19       | 47.98         |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 12       | 47.97         |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 11       | 47.9          |
| (1,114) | 1:519:A:TRP:C | 1:520:A:LYS:N  | 1:520:A:LYS:CA | 1:520:A:LYS:C | 18       | 47.87         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 4        | 47.7          |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 4        | 47.68         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 17       | 47.66         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 15       | 47.51         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 6        | 47.47         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 4        | 47.36         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 8        | 47.33         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 15       | 47.24         |
| (1,11)  | 1:443:A:HIS:C | 1:444:A:SER:N  | 1:444:A:SER:CA | 1:444:A:SER:C | 5        | 47.21         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 7        | 47.05         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 14       | 46.94         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 8        | 46.89         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 1        | 46.83         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 16       | 46.81         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 16       | 46.68         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 1        | 46.57         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 9        | 46.57         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 13       | 46.5          |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 17       | 46.45         |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 17       | 46.41         |
| (1,16)  | 1:446:A:ALA:C | 1:447:A:THR:N  | 1:447:A:THR:CA | 1:447:A:THR:C | 20       | 46.2          |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 6        | 46.11         |
| (1,3)   | 1:438:A:HIS:C | 1:439:A:HIS:N  | 1:439:A:HIS:CA | 1:439:A:HIS:C | 8        | 46.09         |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 19       | 45.86         |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 5        | 45.82         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 19       | 45.77         |
| (1,63)  | 1:487:A:LEU:C | 1:488:A:GLU:N  | 1:488:A:GLU:CA | 1:488:A:GLU:C | 5        | 45.64         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 4        | 45.6          |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 12       | 45.5          |
| (1,43)  | 1:473:A:ASP:N | 1:473:A:ASP:CA | 1:473:A:ASP:C  | 1:474:A:THR:N | 16       | 45.37         |
| (1,11)  | 1:443:A:HIS:C | 1:444:A:SER:N  | 1:444:A:SER:CA | 1:444:A:SER:C | 1        | 45.34         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 16       | 45.33         |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 3        | 45.32         |
| (1,124) | 1:525:A:SER:C | 1:526:A:GLY:N  | 1:526:A:GLY:CA | 1:526:A:GLY:C | 8        | 45.31         |
| (1,9)   | 1:442:A:HIS:C | 1:443:A:HIS:N  | 1:443:A:HIS:CA | 1:443:A:HIS:C | 3        | 45.31         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 19       | 45.28         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 10       | 45.15         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 14       | 45.08         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 19       | 45.02         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 7        | 44.96         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 17       | 44.89         |
| (1,16)  | 1:446:A:ALA:C | 1:447:A:THR:N  | 1:447:A:THR:CA | 1:447:A:THR:C | 18       | 44.74         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 2        | 44.64         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 17       | 44.53         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 2        | 44.4          |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 12       | 44.31         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 3        | 44.14         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 17       | 44.1          |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 20       | 44.02         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 14       | 43.99         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 20       | 43.8          |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 10       | 43.75         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 2        | 43.68         |
| (1,16)  | 1:446:A:ALA:C | 1:447:A:THR:N  | 1:447:A:THR:CA | 1:447:A:THR:C | 13       | 43.47         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 5        | 43.46         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 18       | 43.36         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 19       | 43.34         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 11       | 43.18         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 6        | 43.1          |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 3        | 43.01         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 5        | 43.01         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 10       | 42.68         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 15       | 42.66         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 5        | 42.51         |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 11       | 42.5          |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 9        | 42.43         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 20       | 42.39         |
| (1,95)  | 1:507:A:ILE:N | 1:507:A:ILE:CA | 1:507:A:ILE:C  | 1:508:A:ASN:N | 7        | 42.37         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 8        | 42.31         |
| (1,67)  | 1:489:A:GLY:C | 1:490:A:ASP:N  | 1:490:A:ASP:CA | 1:490:A:ASP:C | 17       | 42.1          |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 18       | 41.73         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 7        | 41.56         |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 8        | 41.41         |
| (1,11)  | 1:443:A:HIS:C | 1:444:A:SER:N  | 1:444:A:SER:CA | 1:444:A:SER:C | 14       | 41.41         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 14       | 41.04         |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 14       | 40.78         |
| (1,3)   | 1:438:A:HIS:C | 1:439:A:HIS:N  | 1:439:A:HIS:CA | 1:439:A:HIS:C | 3        | 40.7          |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 16       | 40.5          |
| (1,57)  | 1:482:A:LEU:N | 1:482:A:LEU:CA | 1:482:A:LEU:C  | 1:483:A:TYR:N | 4        | 40.44         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 2        | 40.26         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 19       | 40.13         |
| (1,16)  | 1:446:A:ALA:C | 1:447:A:THR:N  | 1:447:A:THR:CA | 1:447:A:THR:C | 14       | 40.08         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 13       | 39.95         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 3        | 39.92         |
| (1,9)   | 1:442:A:HIS:C | 1:443:A:HIS:N  | 1:443:A:HIS:CA | 1:443:A:HIS:C | 16       | 39.89         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 15       | 39.83         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 11       | 39.76         |
| (1,12)  | 1:444:A:SER:C | 1:445:A:ASN:N  | 1:445:A:ASN:CA | 1:445:A:ASN:C | 13       | 39.65         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 13       | 39.45         |
| (1,63)  | 1:487:A:LEU:C | 1:488:A:GLU:N  | 1:488:A:GLU:CA | 1:488:A:GLU:C | 19       | 39.43         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 3        | 39.39         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 10       | 39.33         |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 11       | 39.33         |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 6        | 39.25         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 1        | 39.2          |
| (1,16)  | 1:446:A:ALA:C | 1:447:A:THR:N  | 1:447:A:THR:CA | 1:447:A:THR:C | 7        | 39.11         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 8        | 39.01         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 1        | 38.93         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 7        | 38.92         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 14       | 38.89         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 17       | 38.81         |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 7        | 38.73         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 11       | 38.53         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 3        | 38.27         |
| (1,9)   | 1:442:A:HIS:C | 1:443:A:HIS:N  | 1:443:A:HIS:CA | 1:443:A:HIS:C | 8        | 38.2          |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 5        | 38.19         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 18       | 38.08         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 8        | 38.0          |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 4        | 37.89         |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 12       | 37.85         |
| (1,11)  | 1:443:A:HIS:C | 1:444:A:SER:N  | 1:444:A:SER:CA | 1:444:A:SER:C | 9        | 37.81         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 1        | 37.6          |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 7        | 37.37         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 16       | 37.36         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 7        | 37.32         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 16       | 37.26         |
| (1,27)  | 1:460:A:ILE:C | 1:461:A:SER:N  | 1:461:A:SER:CA | 1:461:A:SER:C | 9        | 37.07         |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 6        | 37.07         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 5        | 36.86         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 17       | 36.81         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 19       | 36.64         |
| (1,12)  | 1:444:A:SER:C | 1:445:A:ASN:N  | 1:445:A:ASN:CA | 1:445:A:ASN:C | 15       | 36.41         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 20       | 36.37         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 20       | 36.35         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 16       | 36.29         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 3        | 36.26         |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 16       | 36.11         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 13       | 36.04         |
| (1,3)   | 1:438:A:HIS:C | 1:439:A:HIS:N  | 1:439:A:HIS:CA | 1:439:A:HIS:C | 9        | 35.95         |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 17       | 35.85         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 13       | 35.82         |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 9        | 35.79         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 12       | 35.63         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 16       | 35.35         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 12       | 35.31         |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 13       | 35.17         |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 16       | 35.11         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 15       | 34.99         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 9        | 34.95         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 13       | 34.92         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 9        | 34.9          |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 11       | 34.75         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 9        | 34.74         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 14       | 34.73         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 11       | 34.68         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 20       | 34.65         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 3        | 34.34         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 15       | 34.33         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 19       | 34.31         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 19       | 34.0          |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 16       | 34.0          |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 15       | 34.0          |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 4        | 33.99         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 1        | 33.84         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 20       | 33.82         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 19       | 33.77         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 7        | 33.73         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 20       | 33.68         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 19       | 33.65         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 12       | 33.58         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 6        | 33.54         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 5        | 33.5          |
| (1,81)  | 1:496:A:ARG:C | 1:497:A:PHE:N  | 1:497:A:PHE:CA | 1:497:A:PHE:C | 6        | 33.4          |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 18       | 33.26         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 10       | 33.23         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 8        | 33.22         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 16       | 33.19         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 19       | 33.17         |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 13       | 33.11         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 16       | 32.8          |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 10       | 32.8          |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 17       | 32.74         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 7        | 32.74         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 1        | 32.73         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 14       | 32.69         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 9        | 32.68         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 12       | 32.65         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 12       | 32.6          |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 19       | 32.4          |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 15       | 32.39         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 3        | 32.36         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 13       | 32.36         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 11       | 32.31         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 3        | 32.28         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 10       | 32.25         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 6        | 32.17         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 2        | 32.14         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 20       | 32.11         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 5        | 32.07         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 18       | 32.06         |
| (1,63)  | 1:487:A:LEU:C | 1:488:A:GLU:N  | 1:488:A:GLU:CA | 1:488:A:GLU:C | 10       | 32.04         |
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 12       | 32.02         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 18       | 31.99         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 12       | 31.96         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 9        | 31.91         |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 10       | 31.85         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 20       | 31.76         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 6        | 31.76         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 20       | 31.72         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 6        | 31.67         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 1        | 31.66         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 7        | 31.59         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 16       | 31.56         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 16       | 31.5          |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 17       | 31.46         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 4        | 31.44         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 8        | 31.42         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 17       | 31.4          |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 10       | 31.23         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 12       | 31.15         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 7        | 31.13         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 4        | 31.12         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 8        | 31.03         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 9        | 30.99         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 17       | 30.95         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 8        | 30.92         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 19       | 30.84         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 6        | 30.82         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 10       | 30.81         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 6        | 30.78         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 15       | 30.74         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 2        | 30.65         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 15       | 30.61         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 12       | 30.59         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 11       | 30.48         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 4        | 30.43         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 14       | 30.41         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 20       | 30.37         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 2        | 30.34         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 10       | 30.18         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 11       | 30.13         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 13       | 30.13         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 4        | 30.11         |
| (1,49)  | 1:478:A:ILE:N | 1:478:A:ILE:CA | 1:478:A:ILE:C  | 1:479:A:SER:N | 3        | 30.06         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 8        | 29.98         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 9        | 29.79         |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 10       | 29.77         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 14       | 29.65         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 1        | 29.54         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 7        | 29.46         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 3        | 29.29         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 1        | 29.28         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 16       | 29.25         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 17       | 29.25         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 9        | 29.23         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 2        | 29.21         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 9        | 29.09         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 18       | 29.02         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 20       | 28.9          |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 3        | 28.89         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 12       | 28.8          |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 20       | 28.75         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 2        | 28.74         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 14       | 28.66         |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 16       | 28.66         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 1        | 28.58         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 11       | 28.53         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 2        | 28.41         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 5        | 28.35         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 19       | 28.32         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 15       | 28.25         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 13       | 28.23         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 12       | 28.05         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 14       | 28.0          |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 1        | 27.89         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 13       | 27.81         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 12       | 27.7          |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 8        | 27.62         |
| (1,99)  | 1:509:A:ALA:N | 1:509:A:ALA:CA | 1:509:A:ALA:C  | 1:510:A:TYR:N | 2        | 27.49         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 10       | 27.48         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 6        | 27.35         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 9        | 27.32         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 16       | 27.3          |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 7        | 27.24         |
| (1,17)  | 1:454:A:GLY:C | 1:455:A:VAL:N  | 1:455:A:VAL:CA | 1:455:A:VAL:C | 8        | 27.19         |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 16       | 27.05         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 19       | 27.01         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 19       | 26.91         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 15       | 26.89         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 7        | 26.88         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 1        | 26.81         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 11       | 26.71         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 4        | 26.69         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 15       | 26.46         |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 4        | 26.39         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 7        | 26.07         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 7        | 26.02         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 13       | 25.94         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 2        | 25.85         |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 5        | 25.84         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 16       | 25.8          |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 9        | 25.7          |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 7        | 25.67         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 16       | 25.66         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 4        | 25.49         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 18       | 25.27         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 5        | 25.22         |
| (1,50)  | 1:478:A:ILE:C | 1:479:A:SER:N  | 1:479:A:SER:CA | 1:479:A:SER:C | 15       | 25.15         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 9        | 25.1          |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 15       | 25.06         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 17       | 24.82         |
| (1,28)  | 1:461:A:SER:C | 1:462:A:THR:N  | 1:462:A:THR:CA | 1:462:A:THR:C | 16       | 24.81         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 2        | 24.75         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 17       | 24.56         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 14       | 24.51         |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 12       | 24.51         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 18       | 24.5          |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 4        | 24.44         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 5        | 24.43         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 11       | 24.41         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 18       | 24.12         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 13       | 23.99         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 14       | 23.91         |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 10       | 23.86         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 3        | 23.83         |
| (1,13)  | 1:445:A:ASN:N | 1:445:A:ASN:CA | 1:445:A:ASN:C  | 1:446:A:ALA:N | 15       | 23.7          |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 14       | 23.57         |
| (1,1)   | 1:437:A:MET:C | 1:438:A:HIS:N  | 1:438:A:HIS:CA | 1:438:A:HIS:C | 2        | 23.53         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 9        | 23.49         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 5        | 23.48         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 1        | 23.16         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 15       | 23.13         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 12       | 23.08         |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 12       | 22.98         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 12       | 22.91         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 16       | 22.9          |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 13       | 22.8          |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 10       | 22.75         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 10       | 22.74         |
| (1,12)  | 1:444:A:SER:C | 1:445:A:ASN:N  | 1:445:A:ASN:CA | 1:445:A:ASN:C | 1        | 22.72         |
| (1,58)  | 1:482:A:LEU:C | 1:483:A:TYR:N  | 1:483:A:TYR:CA | 1:483:A:TYR:C | 16       | 22.61         |
| (1,16)  | 1:446:A:ALA:C | 1:447:A:THR:N  | 1:447:A:THR:CA | 1:447:A:THR:C | 2        | 22.58         |
| (1,102) | 1:512:A:GLU:N | 1:512:A:GLU:CA | 1:512:A:GLU:C  | 1:513:A:ILE:N | 2        | 22.33         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 8        | 22.13         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 10       | 22.11         |
| (1,112) | 1:518:A:CYS:C | 1:519:A:TRP:N  | 1:519:A:TRP:CA | 1:519:A:TRP:C | 9        | 22.1          |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 9        | 22.07         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 17       | 22.02         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 6        | 21.99         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 20       | 21.88         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 20       | 21.87         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 6        | 21.84         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 2        | 21.79         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 17       | 21.78         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 4        | 21.76         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 19       | 21.72         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 9        | 21.66         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 5        | 21.63         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 2        | 21.46         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 13       | 21.24         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 18       | 21.09         |
| (1,12)  | 1:444:A:SER:C | 1:445:A:ASN:N  | 1:445:A:ASN:CA | 1:445:A:ASN:C | 2        | 21.05         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 3        | 20.95         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 11       | 20.83         |
| (1,31)  | 1:463:A:GLU:N | 1:463:A:GLU:CA | 1:463:A:GLU:C  | 1:464:A:PRO:N | 13       | 20.66         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 5        | 20.57         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 4        | 20.45         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 4        | 20.45         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 9        | 20.43         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 10       | 20.35         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 8        | 20.29         |
| (1,64)  | 1:488:A:GLU:N | 1:488:A:GLU:CA | 1:488:A:GLU:C  | 1:489:A:GLY:N | 19       | 20.29         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 9        | 20.19         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 18       | 20.19         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 18       | 20.06         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 1        | 19.97         |
| (1,69)  | 1:490:A:ASP:C | 1:491:A:THR:N  | 1:491:A:THR:CA | 1:491:A:THR:C | 11       | 19.96         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 4        | 19.9          |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 7        | 19.85         |
| (1,9)   | 1:442:A:HIS:C | 1:443:A:HIS:N  | 1:443:A:HIS:CA | 1:443:A:HIS:C | 9        | 19.83         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 17       | 19.75         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 1        | 19.74         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 14       | 19.73         |
| (1,11)  | 1:443:A:HIS:C | 1:444:A:SER:N  | 1:444:A:SER:CA | 1:444:A:SER:C | 20       | 19.71         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 19       | 19.65         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 18       | 19.55         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 6        | 19.53         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 1        | 19.47         |
| (1,12)  | 1:444:A:SER:C | 1:445:A:ASN:N  | 1:445:A:ASN:CA | 1:445:A:ASN:C | 5        | 19.43         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 17       | 19.34         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 19       | 19.33         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 6        | 19.32         |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 2        | 19.28         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 4        | 19.25         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 19       | 19.05         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 10       | 19.04         |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 15       | 19.04         |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 2        | 18.92         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 9        | 18.82         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 16       | 18.77         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 13       | 18.7          |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 10       | 18.67         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 12       | 18.65         |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 11       | 18.6          |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 11       | 18.57         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 13       | 18.52         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 15       | 18.44         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 4        | 18.43         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 3        | 18.34         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 3        | 18.24         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 8        | 18.24         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 7        | 18.13         |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 12       | 17.95         |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 6        | 17.93         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 1        | 17.8          |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 10       | 17.76         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 16       | 17.65         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 1        | 17.57         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 6        | 17.51         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 18       | 17.46         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 19       | 17.39         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 12       | 17.32         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 8        | 17.22         |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 15       | 17.13         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 20       | 17.12         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 14       | 17.1          |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 4        | 17.08         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 2        | 17.07         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 6        | 16.95         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 5        | 16.54         |
| (1,34)  | 1:464:A:PRO:C | 1:465:A:LEU:N  | 1:465:A:LEU:CA | 1:465:A:LEU:C | 16       | 16.48         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 9        | 16.43         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 8        | 16.25         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 11       | 16.2          |
| (1,101) | 1:510:A:TYR:N | 1:510:A:TYR:CA | 1:510:A:TYR:C  | 1:511:A:THR:N | 3        | 15.99         |
| (1,7)   | 1:440:A:HIS:C | 1:441:A:HIS:N  | 1:441:A:HIS:CA | 1:441:A:HIS:C | 17       | 15.97         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 4        | 15.9          |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 5        | 15.87         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 13       | 15.87         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 5        | 15.73         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 15       | 15.73         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 6        | 15.71         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 11       | 15.7          |
| (1,55)  | 1:481:A:VAL:N | 1:481:A:VAL:CA | 1:481:A:VAL:C  | 1:482:A:LEU:N | 18       | 15.6          |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 17       | 15.55         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 13       | 15.4          |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 16       | 15.38         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 17       | 15.35         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 1        | 15.32         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 11       | 15.24         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 10       | 15.23         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 6        | 15.19         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 8        | 15.16         |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 5        | 15.13         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 3        | 15.02         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 2        | 15.0          |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 19       | 14.99         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 18       | 14.97         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 4        | 14.91         |
| (1,120) | 1:522:A:GLU:C | 1:523:A:ILE:N  | 1:523:A:ILE:CA | 1:523:A:ILE:C | 13       | 14.85         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 12       | 14.78         |
| (1,135) | 1:531:A:ARG:N | 1:531:A:ARG:CA | 1:531:A:ARG:C  | 1:532:A:TYR:N | 14       | 14.75         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 14       | 14.71         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 14       | 14.62         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 20       | 14.58         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 20       | 14.5          |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 20       | 14.34         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 2        | 14.33         |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 11       | 14.17         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 13       | 14.14         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 11       | 14.02         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 4        | 13.94         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 16       | 13.92         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 8        | 13.91         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 19       | 13.84         |
| (1,47)  | 1:476:A:ALA:N | 1:476:A:ALA:CA | 1:476:A:ALA:C  | 1:477:A:ALA:N | 7        | 13.81         |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 10       | 13.77         |
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 9        | 13.75         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 2        | 13.72         |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 5        | 13.68         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 3        | 13.63         |
| (1,14)  | 1:445:A:ASN:C | 1:446:A:ALA:N  | 1:446:A:ALA:CA | 1:446:A:ALA:C | 18       | 13.46         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 15       | 13.34         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 12       | 13.34         |
| (1,77)  | 1:494:A:HIS:C | 1:495:A:ALA:N  | 1:495:A:ALA:CA | 1:495:A:ALA:C | 7        | 13.19         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 10       | 13.14         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 11       | 12.7          |
| (1,108) | 1:516:A:LYS:N | 1:516:A:LYS:CA | 1:516:A:LYS:C  | 1:517:A:HIS:N | 2        | 12.66         |
| (1,12)  | 1:444:A:SER:C | 1:445:A:ASN:N  | 1:445:A:ASN:CA | 1:445:A:ASN:C | 12       | 12.66         |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 6        | 12.66         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 5        | 12.6          |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 16       | 12.58         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 15       | 12.46         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 19       | 12.38         |
| (1,15)  | 1:446:A:ALA:N | 1:446:A:ALA:CA | 1:446:A:ALA:C  | 1:447:A:THR:N | 6        | 12.33         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 14       | 12.32         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 12       | 12.25         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 16       | 12.17         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 3        | 11.89         |
| (1,29)  | 1:462:A:THR:N | 1:462:A:THR:CA | 1:462:A:THR:C  | 1:463:A:GLU:N | 20       | 11.65         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 15       | 11.61         |
| (1,12)  | 1:444:A:SER:C | 1:445:A:ASN:N  | 1:445:A:ASN:CA | 1:445:A:ASN:C | 18       | 11.53         |
| (1,79)  | 1:495:A:ALA:C | 1:496:A:ARG:N  | 1:496:A:ARG:CA | 1:496:A:ARG:C | 20       | 11.47         |
| (1,32)  | 1:463:A:GLU:C | 1:464:A:PRO:N  | 1:464:A:PRO:CA | 1:464:A:PRO:C | 9        | 11.4          |

Continued on next page...

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 13       | 11.36         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 2        | 11.29         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 20       | 11.25         |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 9        | 11.25         |
| (1,51)  | 1:479:A:SER:N | 1:479:A:SER:CA | 1:479:A:SER:C  | 1:480:A:GLU:N | 8        | 11.19         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 1        | 11.1          |
| (1,5)   | 1:439:A:HIS:C | 1:440:A:HIS:N  | 1:440:A:HIS:CA | 1:440:A:HIS:C | 3        | 11.06         |
| (1,11)  | 1:443:A:HIS:C | 1:444:A:SER:N  | 1:444:A:SER:CA | 1:444:A:SER:C | 7        | 10.96         |
| (1,108) | 1:516:A:LYS:N | 1:516:A:LYS:CA | 1:516:A:LYS:C  | 1:517:A:HIS:N | 6        | 10.92         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 17       | 10.92         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 17       | 10.91         |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 15       | 10.83         |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 18       | 10.75         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 7        | 10.68         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 6        | 10.67         |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 3        | 10.52         |
| (1,3)   | 1:438:A:HIS:C | 1:439:A:HIS:N  | 1:439:A:HIS:CA | 1:439:A:HIS:C | 7        | 10.5          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 15       | 10.26         |
| (1,108) | 1:516:A:LYS:N | 1:516:A:LYS:CA | 1:516:A:LYS:C  | 1:517:A:HIS:N | 20       | 10.22         |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 11       | 10.2          |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 18       | 10.18         |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 1        | 10.14         |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 15       | 10.1          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 9        | 9.96          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 15       | 9.93          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 2        | 9.91          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 18       | 9.89          |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 8        | 9.89          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 1        | 9.87          |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 6        | 9.85          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 4        | 9.82          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 10       | 9.8           |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 20       | 9.7           |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 5        | 9.65          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 6        | 9.63          |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 8        | 9.59          |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 2        | 9.58          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 7        | 9.57          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 11       | 9.56          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 10       | 9.53          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 12       | 9.53          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 16       | 9.53          |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 20       | 9.53          |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 14       | 9.51          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 9        | 9.38          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 20       | 9.38          |
| (1,29)  | 1:462:A:THR:N | 1:462:A:THR:CA | 1:462:A:THR:C  | 1:463:A:GLU:N | 2        | 9.37          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 12       | 9.36          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 18       | 9.34          |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 12       | 9.33          |
| (1,108) | 1:516:A:LYS:N | 1:516:A:LYS:CA | 1:516:A:LYS:C  | 1:517:A:HIS:N | 7        | 9.32          |

Continued on next page...

*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,107) | 1:515:A:LYS:C | 1:516:A:LYS:N  | 1:516:A:LYS:CA | 1:516:A:LYS:C | 17       | 9.31          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 6        | 9.27          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 2        | 9.26          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 7        | 9.19          |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 16       | 9.16          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 12       | 9.15          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 14       | 9.13          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 18       | 9.13          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 11       | 9.08          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 19       | 9.08          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 2        | 9.04          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 13       | 9.03          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 14       | 9.03          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 16       | 8.98          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 6        | 8.89          |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 17       | 8.89          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 1        | 8.85          |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 9        | 8.79          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 17       | 8.66          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 8        | 8.53          |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 7        | 8.53          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 15       | 8.52          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 5        | 8.47          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 13       | 8.47          |
| (1,3)   | 1:438:A:HIS:C | 1:439:A:HIS:N  | 1:439:A:HIS:CA | 1:439:A:HIS:C | 14       | 8.47          |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 11       | 8.46          |
| (1,108) | 1:516:A:LYS:N | 1:516:A:LYS:CA | 1:516:A:LYS:C  | 1:517:A:HIS:N | 5        | 8.45          |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 5        | 8.31          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 4        | 8.25          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 17       | 8.24          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 3        | 8.21          |
| (1,131) | 1:529:A:GLU:N | 1:529:A:GLU:CA | 1:529:A:GLU:C  | 1:530:A:GLN:N | 20       | 8.18          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 19       | 8.05          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 10       | 8.0           |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 8        | 7.99          |
| (1,111) | 1:517:A:HIS:C | 1:518:A:CYS:N  | 1:518:A:CYS:CA | 1:518:A:CYS:C | 3        | 7.94          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 7        | 7.91          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 15       | 7.87          |
| (1,111) | 1:517:A:HIS:C | 1:518:A:CYS:N  | 1:518:A:CYS:CA | 1:518:A:CYS:C | 9        | 7.69          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 2        | 7.62          |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 17       | 7.6           |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 7        | 7.57          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 11       | 7.45          |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 8        | 7.27          |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 7        | 7.23          |
| (1,11)  | 1:443:A:HIS:C | 1:444:A:SER:N  | 1:444:A:SER:CA | 1:444:A:SER:C | 8        | 7.23          |
| (1,86)  | 1:499:A:THR:C | 1:500:A:PRO:N  | 1:500:A:PRO:CA | 1:500:A:PRO:C | 10       | 7.13          |
| (1,22)  | 1:457:A:VAL:C | 1:458:A:LYS:N  | 1:458:A:LYS:CA | 1:458:A:LYS:C | 3        | 7.09          |
| (1,3)   | 1:438:A:HIS:C | 1:439:A:HIS:N  | 1:439:A:HIS:CA | 1:439:A:HIS:C | 15       | 7.09          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 7        | 6.91          |
| (1,2)   | 1:438:A:HIS:N | 1:438:A:HIS:CA | 1:438:A:HIS:C  | 1:439:A:HIS:N | 1        | 6.89          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 8        | 6.82          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 16       | 6.64          |
| (1,51)  | 1:479:A:SER:N | 1:479:A:SER:CA | 1:479:A:SER:C  | 1:480:A:GLU:N | 10       | 6.63          |
| (1,106) | 1:515:A:LYS:N | 1:515:A:LYS:CA | 1:515:A:LYS:C  | 1:516:A:LYS:N | 17       | 6.55          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 8        | 6.38          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 5        | 6.28          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 9        | 6.27          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 3        | 6.22          |
| (1,51)  | 1:479:A:SER:N | 1:479:A:SER:CA | 1:479:A:SER:C  | 1:480:A:GLU:N | 5        | 6.21          |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 14       | 6.18          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 18       | 6.16          |
| (1,108) | 1:516:A:LYS:N | 1:516:A:LYS:CA | 1:516:A:LYS:C  | 1:517:A:HIS:N | 4        | 6.12          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 3        | 6.12          |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 1        | 6.09          |
| (1,111) | 1:517:A:HIS:C | 1:518:A:CYS:N  | 1:518:A:CYS:CA | 1:518:A:CYS:C | 8        | 5.99          |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 5        | 5.96          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 5        | 5.83          |
| (1,51)  | 1:479:A:SER:N | 1:479:A:SER:CA | 1:479:A:SER:C  | 1:480:A:GLU:N | 11       | 5.83          |
| (1,11)  | 1:443:A:HIS:C | 1:444:A:SER:N  | 1:444:A:SER:CA | 1:444:A:SER:C | 11       | 5.63          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 4        | 5.61          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 3        | 5.6           |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 19       | 5.6           |
| (1,6)   | 1:440:A:HIS:N | 1:440:A:HIS:CA | 1:440:A:HIS:C  | 1:441:A:HIS:N | 2        | 5.55          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 10       | 5.5           |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 12       | 5.49          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 8        | 5.47          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 11       | 5.44          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 14       | 5.43          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 20       | 5.4           |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 15       | 5.38          |
| (1,29)  | 1:462:A:THR:N | 1:462:A:THR:CA | 1:462:A:THR:C  | 1:463:A:GLU:N | 12       | 5.38          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 16       | 5.37          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 8        | 5.33          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 20       | 5.29          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 17       | 5.24          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 15       | 5.21          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 13       | 5.2           |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 1        | 5.2           |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 12       | 5.18          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 5        | 5.17          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 13       | 5.12          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 19       | 5.12          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 9        | 5.06          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 2        | 5.05          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 2        | 5.03          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 4        | 5.03          |
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 6        | 5.03          |
| (1,8)   | 1:441:A:HIS:N | 1:441:A:HIS:CA | 1:441:A:HIS:C  | 1:442:A:HIS:N | 4        | 5.0           |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 1        | 4.96          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 10       | 4.95          |
| (1,105) | 1:514:A:ASN:C | 1:515:A:LYS:N  | 1:515:A:LYS:CA | 1:515:A:LYS:C | 17       | 4.94          |

*Continued on next page...*

Continued from previous page...

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,70)  | 1:491:A:THR:N | 1:491:A:THR:CA | 1:491:A:THR:C  | 1:492:A:GLU:N | 17       | 4.87          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 14       | 4.82          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 11       | 4.79          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 20       | 4.78          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 13       | 4.7           |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 14       | 4.63          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 9        | 4.62          |
| (1,16)  | 1:446:A:ALA:C | 1:447:A:THR:N  | 1:447:A:THR:CA | 1:447:A:THR:C | 5        | 4.61          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 8        | 4.59          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 15       | 4.59          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 12       | 4.57          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 19       | 4.56          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 17       | 4.53          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 9        | 4.52          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 17       | 4.51          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 7        | 4.48          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 1        | 4.48          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 6        | 4.43          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 7        | 4.43          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 16       | 4.43          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 14       | 4.41          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 12       | 4.39          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 19       | 4.39          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 20       | 4.38          |
| (1,51)  | 1:479:A:SER:N | 1:479:A:SER:CA | 1:479:A:SER:C  | 1:480:A:GLU:N | 2        | 4.35          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 18       | 4.31          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 4        | 4.29          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 3        | 4.27          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 2        | 4.27          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 17       | 4.25          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 2        | 4.24          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 3        | 4.18          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 11       | 4.17          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 1        | 4.12          |
| (1,29)  | 1:462:A:THR:N | 1:462:A:THR:CA | 1:462:A:THR:C  | 1:463:A:GLU:N | 15       | 4.12          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 3        | 4.09          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 18       | 4.07          |
| (1,108) | 1:516:A:LYS:N | 1:516:A:LYS:CA | 1:516:A:LYS:C  | 1:517:A:HIS:N | 19       | 4.03          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 9        | 4.0           |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 13       | 3.98          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 5        | 3.91          |
| (1,51)  | 1:479:A:SER:N | 1:479:A:SER:CA | 1:479:A:SER:C  | 1:480:A:GLU:N | 16       | 3.9           |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 5        | 3.87          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 18       | 3.83          |
| (1,130) | 1:528:A:HIS:C | 1:529:A:GLU:N  | 1:529:A:GLU:CA | 1:529:A:GLU:C | 16       | 3.81          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 6        | 3.8           |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 16       | 3.74          |
| (1,111) | 1:517:A:HIS:C | 1:518:A:CYS:N  | 1:518:A:CYS:CA | 1:518:A:CYS:C | 15       | 3.68          |
| (1,108) | 1:516:A:LYS:N | 1:516:A:LYS:CA | 1:516:A:LYS:C  | 1:517:A:HIS:N | 11       | 3.67          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 10       | 3.62          |
| (1,60)  | 1:484:A:VAL:C | 1:485:A:ASP:N  | 1:485:A:ASP:CA | 1:485:A:ASP:C | 17       | 3.59          |

Continued on next page...

*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 13       | 3.56          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 20       | 3.46          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 6        | 3.45          |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 5        | 3.4           |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 12       | 3.38          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 4        | 3.37          |
| (1,111) | 1:517:A:HIS:C | 1:518:A:CYS:N  | 1:518:A:CYS:CA | 1:518:A:CYS:C | 4        | 3.36          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 12       | 3.32          |
| (1,129) | 1:528:A:HIS:N | 1:528:A:HIS:CA | 1:528:A:HIS:C  | 1:529:A:GLU:N | 11       | 3.31          |
| (1,9)   | 1:442:A:HIS:C | 1:443:A:HIS:N  | 1:443:A:HIS:CA | 1:443:A:HIS:C | 6        | 3.31          |
| (1,83)  | 1:497:A:PHE:C | 1:498:A:LYS:N  | 1:498:A:LYS:CA | 1:498:A:LYS:C | 7        | 3.3           |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 1        | 3.21          |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 15       | 3.18          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 3        | 3.12          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 14       | 3.11          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 7        | 3.1           |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 17       | 2.98          |
| (1,105) | 1:514:A:ASN:C | 1:515:A:LYS:N  | 1:515:A:LYS:CA | 1:515:A:LYS:C | 12       | 2.96          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 12       | 2.8           |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 19       | 2.8           |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 18       | 2.79          |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 3        | 2.77          |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 9        | 2.75          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 18       | 2.74          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 19       | 2.71          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 4        | 2.57          |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 6        | 2.52          |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 8        | 2.38          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 16       | 2.33          |
| (1,66)  | 1:489:A:GLY:N | 1:489:A:GLY:CA | 1:489:A:GLY:C  | 1:490:A:ASP:N | 13       | 2.32          |
| (1,19)  | 1:455:A:VAL:C | 1:456:A:ILE:N  | 1:456:A:ILE:CA | 1:456:A:ILE:C | 20       | 2.29          |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 10       | 2.26          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 5        | 2.23          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 19       | 2.19          |
| (1,111) | 1:517:A:HIS:C | 1:518:A:CYS:N  | 1:518:A:CYS:CA | 1:518:A:CYS:C | 16       | 2.18          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 4        | 2.17          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 1        | 2.11          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 20       | 2.09          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 15       | 2.08          |
| (1,133) | 1:530:A:GLN:N | 1:530:A:GLN:CA | 1:530:A:GLN:C  | 1:531:A:ARG:N | 16       | 2.08          |
| (1,89)  | 1:501:A:GLU:N | 1:501:A:GLU:CA | 1:501:A:GLU:C  | 1:502:A:ASP:N | 4        | 2.07          |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 11       | 2.03          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 9        | 2.02          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 13       | 1.92          |
| (1,51)  | 1:479:A:SER:N | 1:479:A:SER:CA | 1:479:A:SER:C  | 1:480:A:GLU:N | 18       | 1.92          |
| (1,104) | 1:514:A:ASN:N | 1:514:A:ASN:CA | 1:514:A:ASN:C  | 1:515:A:LYS:N | 12       | 1.91          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 6        | 1.88          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 15       | 1.86          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 8        | 1.82          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 3        | 1.77          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 10       | 1.77          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,10)  | 1:443:A:HIS:N | 1:443:A:HIS:CA | 1:443:A:HIS:C  | 1:444:A:SER:N | 18       | 1.71          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 2        | 1.69          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 17       | 1.61          |
| (1,4)   | 1:439:A:HIS:N | 1:439:A:HIS:CA | 1:439:A:HIS:C  | 1:440:A:HIS:N | 2        | 1.51          |
| (1,126) | 1:526:A:GLY:C | 1:527:A:ASP:N  | 1:527:A:ASP:CA | 1:527:A:ASP:C | 17       | 1.42          |
| (1,108) | 1:516:A:LYS:N | 1:516:A:LYS:CA | 1:516:A:LYS:C  | 1:517:A:HIS:N | 18       | 1.33          |
| (1,128) | 1:527:A:ASP:C | 1:528:A:HIS:N  | 1:528:A:HIS:CA | 1:528:A:HIS:C | 11       | 1.25          |
| (1,33)  | 1:464:A:PRO:N | 1:464:A:PRO:CA | 1:464:A:PRO:C  | 1:465:A:LEU:N | 13       | 1.21          |
| (1,51)  | 1:479:A:SER:N | 1:479:A:SER:CA | 1:479:A:SER:C  | 1:480:A:GLU:N | 12       | 1.12          |