



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 03:33 PM UTC

PDB ID : 2LOP / pdb\_00002lop  
BMRB ID : 18220  
Title : Backbone structure of human membrane protein TMEM14A  
Authors : Eichmann, C.; Klammt, C.; Maslennikov, I.; Kwiatkowski, W.; Riek, R.; Choe, S.  
Deposited on : 2012-01-26

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

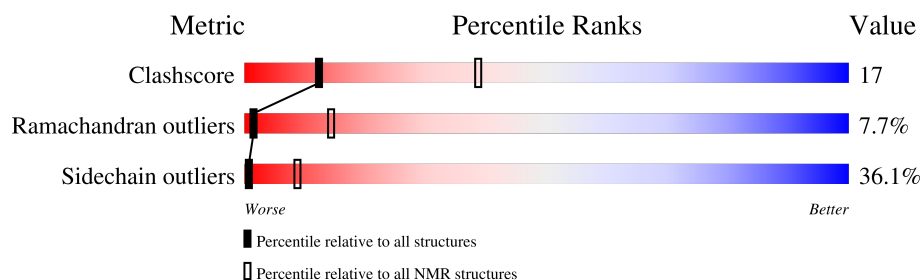
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 64%.

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     | 108    | <div> <div></div> <div>27%</div> <div>42%</div> <div>6%</div> <div>18%</div> <div>8%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:7-A:49, A:53-A:68, A:79-A:99 (80) | 1.66              | 4            |

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 4 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1569 atoms, of which 817 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transmembrane protein 14A.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 99       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1569  | 500 | 817 | 127 | 119 | 6 |       |

There are 9 discrepancies between the modelled and reference sequences:

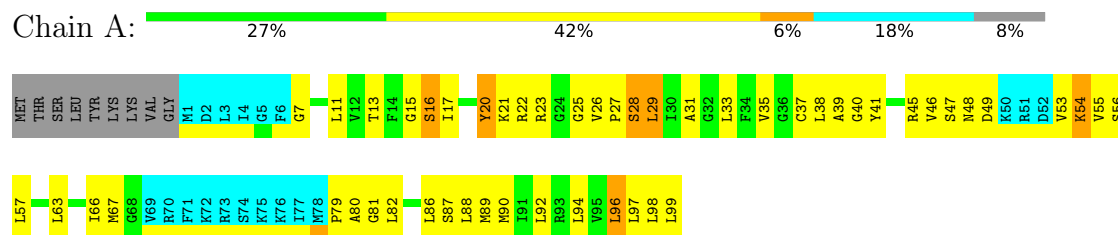
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -8      | MET      | -      | expression tag | UNP Q9Y6G1 |
| A     | -7      | THR      | -      | expression tag | UNP Q9Y6G1 |
| A     | -6      | SER      | -      | expression tag | UNP Q9Y6G1 |
| A     | -5      | LEU      | -      | expression tag | UNP Q9Y6G1 |
| A     | -4      | TYR      | -      | expression tag | UNP Q9Y6G1 |
| A     | -3      | LYS      | -      | expression tag | UNP Q9Y6G1 |
| A     | -2      | LYS      | -      | expression tag | UNP Q9Y6G1 |
| A     | -1      | VAL      | -      | expression tag | UNP Q9Y6G1 |
| A     | 0       | GLY      | -      | expression tag | UNP Q9Y6G1 |

## 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: Transmembrane protein 14A

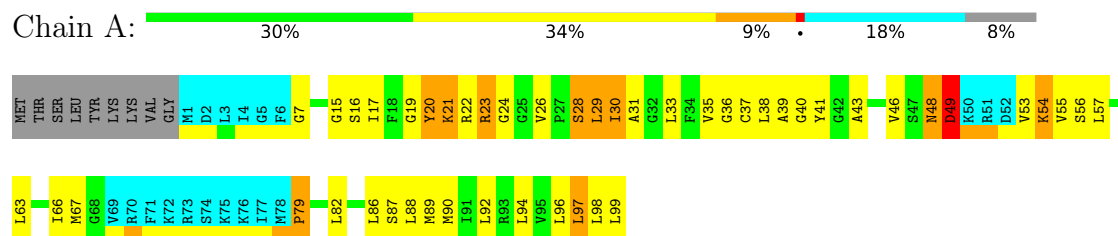


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

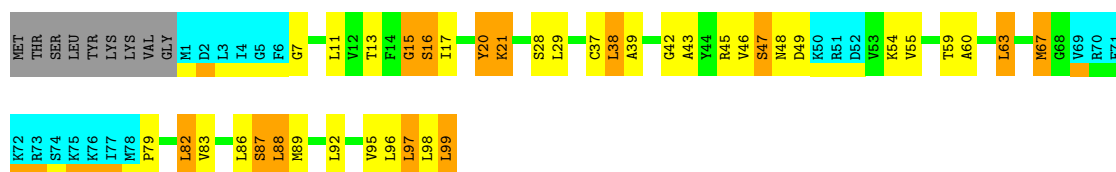
- Molecule 1: Transmembrane protein 14A



#### 4.2.2 Score per residue for model 2

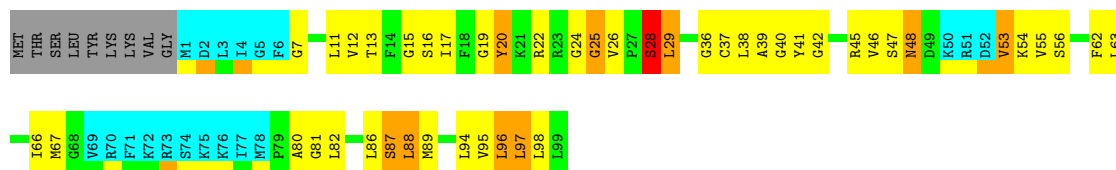
- Molecule 1: Transmembrane protein 14A





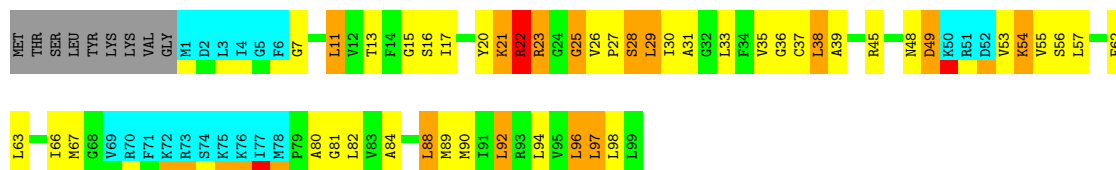
### 4.2.3 Score per residue for model 3

- Molecule 1: Transmembrane protein 14A



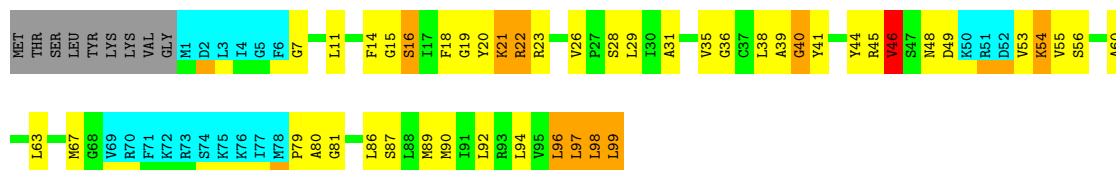
### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Transmembrane protein 14A



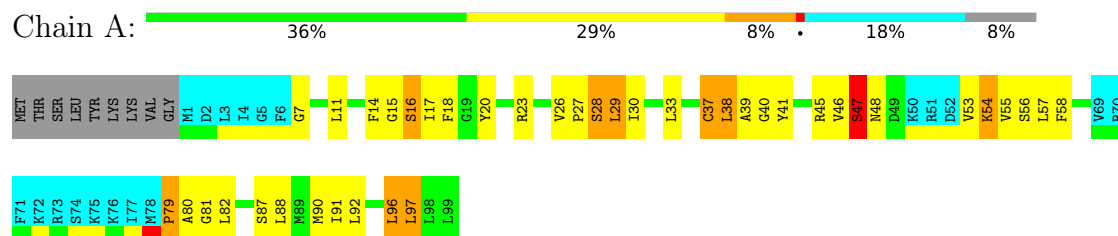
### 4.2.5 Score per residue for model 5

- Molecule 1: Transmembrane protein 14A



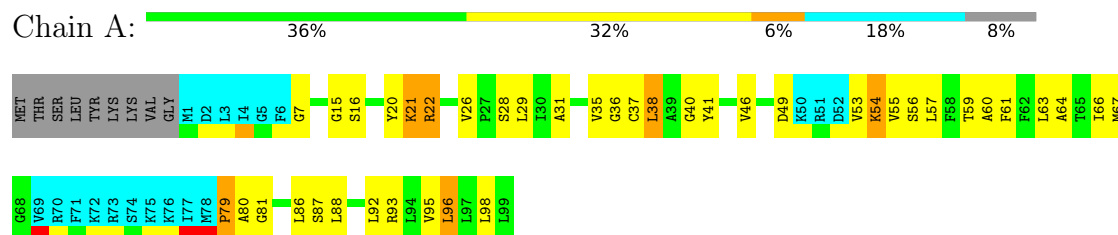
### 4.2.6 Score per residue for model 6

- Molecule 1: Transmembrane protein 14A



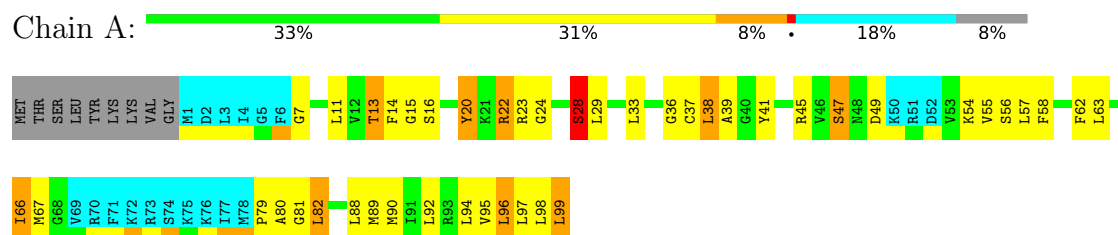
#### 4.2.7 Score per residue for model 7

- Molecule 1: Transmembrane protein 14A



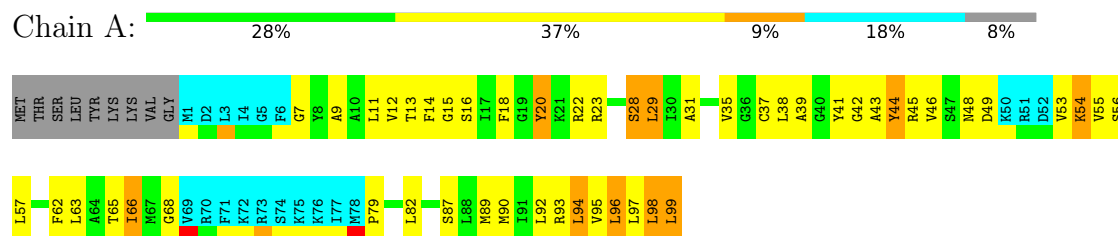
#### 4.2.8 Score per residue for model 8

- Molecule 1: Transmembrane protein 14A



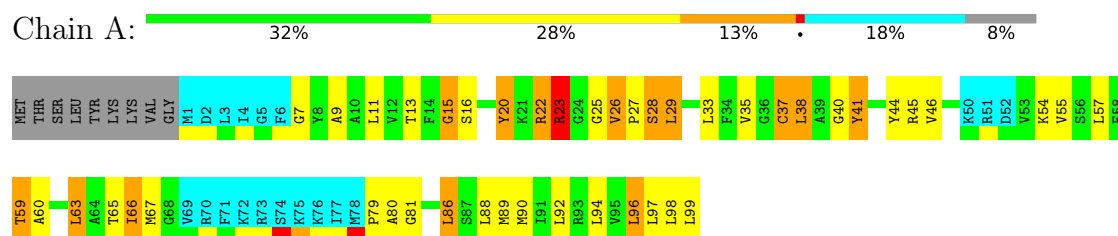
#### 4.2.9 Score per residue for model 9

- Molecule 1: Transmembrane protein 14A



### 4.2.10 Score per residue for model 10

- Molecule 1: Transmembrane protein 14A



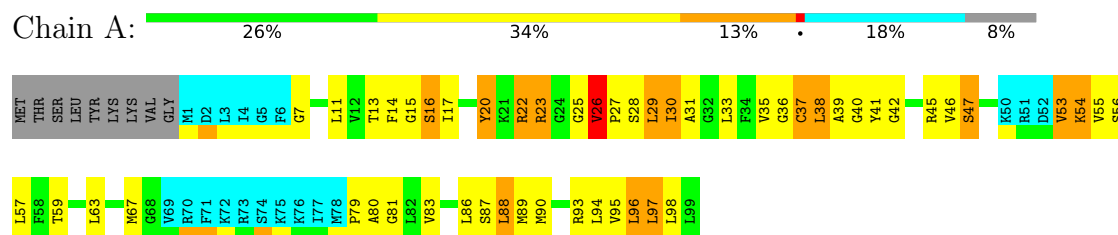
### 4.2.11 Score per residue for model 11

- Molecule 1: Transmembrane protein 14A



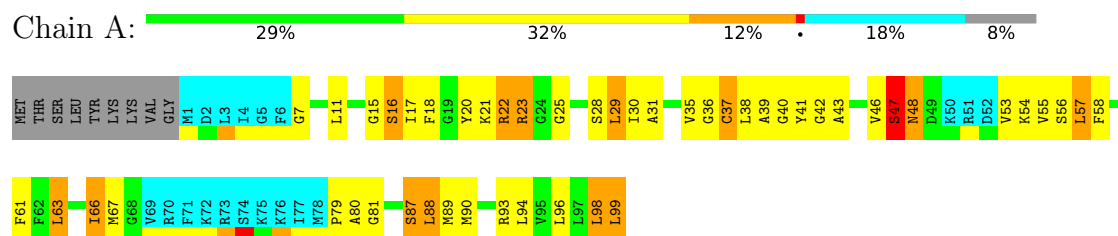
### 4.2.12 Score per residue for model 12

- Molecule 1: Transmembrane protein 14A



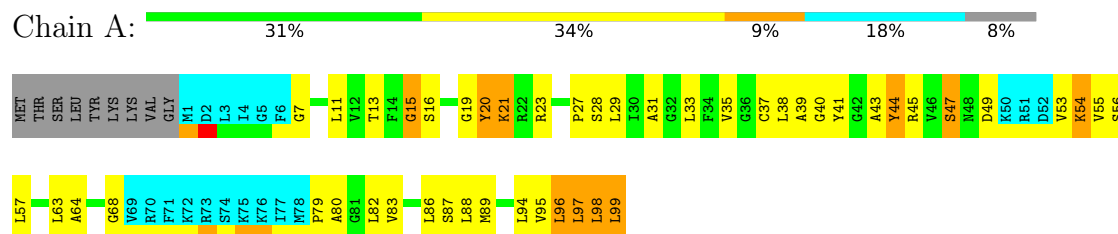
### 4.2.13 Score per residue for model 13

- Molecule 1: Transmembrane protein 14A



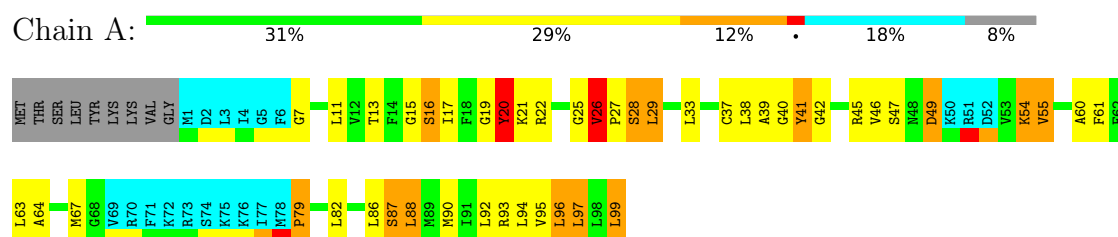
## 4.2.14 Score per residue for model 14

- Molecule 1: Transmembrane protein 14A



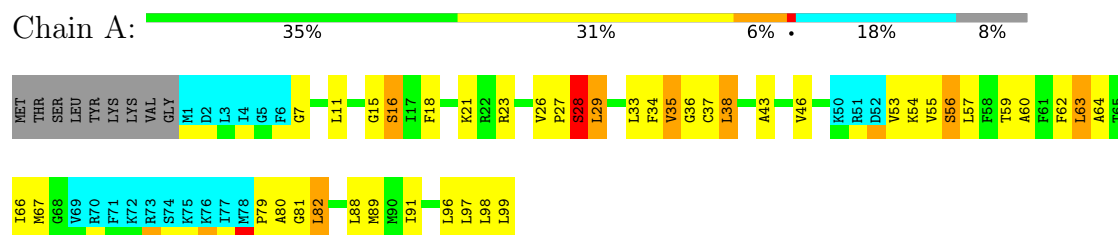
## 4.2.15 Score per residue for model 15

- Molecule 1: Transmembrane protein 14A



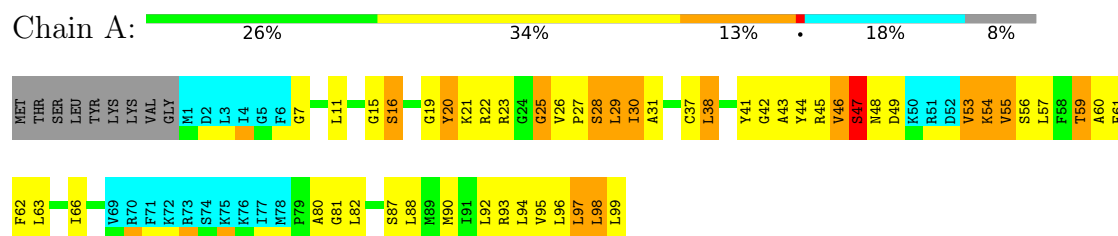
## 4.2.16 Score per residue for model 16

- Molecule 1: Transmembrane protein 14A



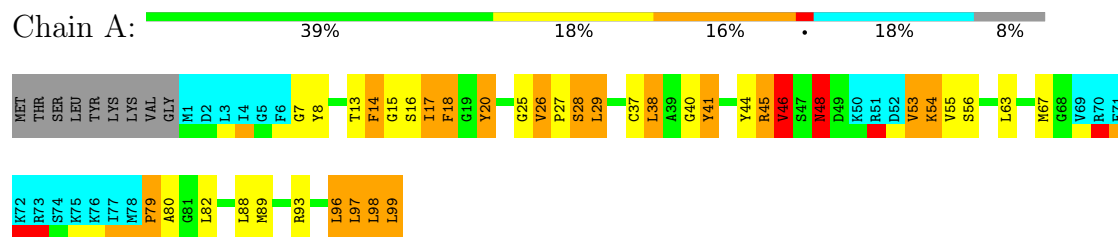
## 4.2.17 Score per residue for model 17

- Molecule 1: Transmembrane protein 14A



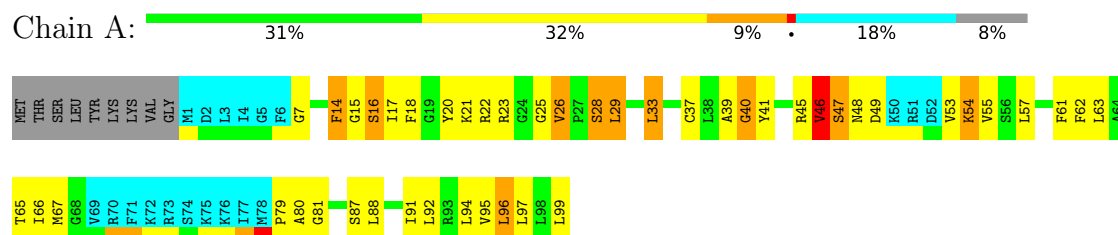
### 4.2.18 Score per residue for model 18

- Molecule 1: Transmembrane protein 14A



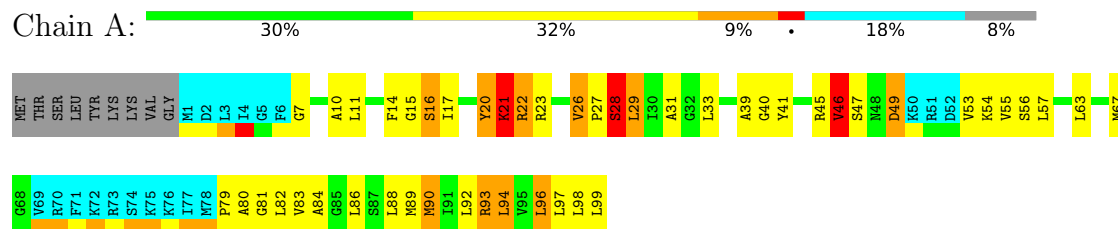
### 4.2.19 Score per residue for model 19

- Molecule 1: Transmembrane protein 14A



### 4.2.20 Score per residue for model 20

- Molecule 1: Transmembrane protein 14A



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution |         |
| CYANA         | 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                       | 819            |
| Number of shifts mapped to atoms             | 819            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 64%            |

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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 [i](#)

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     | 588   | 632      | 632      | 21±3    |
| All | All   | 11760 | 12640    | 12640    | 416     |

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 17.

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

| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:63:LEU:O   | 1:A:66:ILE:HG22 | 0.84     | 1.70        | 10     | 3     |
| 1:A:80:ALA:O   | 1:A:83:VAL:HG22 | 0.84     | 1.72        | 20     | 2     |
| 1:A:88:LEU:O   | 1:A:92:LEU:HD12 | 0.83     | 1.73        | 4      | 1     |
| 1:A:62:PHE:CD2 | 1:A:66:ILE:HD11 | 0.82     | 2.09        | 4      | 3     |
| 1:A:62:PHE:O   | 1:A:66:ILE:HD12 | 0.82     | 1.72        | 9      | 1     |
| 1:A:31:ALA:O   | 1:A:35:VAL:HG22 | 0.78     | 1.77        | 9      | 2     |
| 1:A:60:ALA:HB1 | 1:A:82:LEU:HD21 | 0.77     | 1.56        | 2      | 1     |
| 1:A:45:ARG:O   | 1:A:46:VAL:HG13 | 0.76     | 1.79        | 19     | 1     |
| 1:A:26:VAL:O   | 1:A:31:ALA:HB2  | 0.74     | 1.82        | 20     | 1     |
| 1:A:82:LEU:C   | 1:A:82:LEU:HD12 | 0.73     | 2.08        | 16     | 1     |
| 1:A:45:ARG:C   | 1:A:46:VAL:HG12 | 0.71     | 2.10        | 20     | 2     |
| 1:A:45:ARG:C   | 1:A:46:VAL:HG22 | 0.71     | 2.10        | 19     | 1     |
| 1:A:31:ALA:O   | 1:A:35:VAL:HG23 | 0.71     | 1.85        | 4      | 3     |
| 1:A:62:PHE:CE2 | 1:A:66:ILE:HD11 | 0.67     | 2.24        | 17     | 3     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:55:VAL:O    | 1:A:59:THR:HG23 | 0.67     | 1.89        | 7      | 1     |
| 1:A:61:PHE:O    | 1:A:65:THR:HG23 | 0.66     | 1.90        | 19     | 1     |
| 1:A:53:VAL:HG22 | 1:A:53:VAL:O    | 0.66     | 1.89        | 12     | 1     |
| 1:A:25:GLY:O    | 1:A:26:VAL:HG23 | 0.66     | 1.91        | 12     | 2     |
| 1:A:30:ILE:HD12 | 1:A:31:ALA:N    | 0.65     | 2.07        | 13     | 1     |
| 1:A:63:LEU:HA   | 1:A:66:ILE:HD12 | 0.65     | 1.68        | 16     | 1     |
| 1:A:45:ARG:O    | 1:A:46:VAL:HG23 | 0.65     | 1.91        | 5      | 1     |
| 1:A:26:VAL:O    | 1:A:26:VAL:HG12 | 0.62     | 1.93        | 1      | 1     |
| 1:A:46:VAL:O    | 1:A:46:VAL:HG22 | 0.62     | 1.93        | 20     | 1     |
| 1:A:86:LEU:C    | 1:A:86:LEU:HD13 | 0.60     | 2.21        | 1      | 1     |
| 1:A:35:VAL:HG13 | 1:A:59:THR:HG21 | 0.60     | 1.74        | 16     | 1     |
| 1:A:44:TYR:CE2  | 1:A:49:ASP:O    | 0.60     | 2.55        | 9      | 1     |
| 1:A:87:SER:O    | 1:A:91:ILE:HD12 | 0.60     | 1.97        | 6      | 1     |
| 1:A:62:PHE:O    | 1:A:66:ILE:HG23 | 0.59     | 1.97        | 11     | 1     |
| 1:A:86:LEU:HD13 | 1:A:86:LEU:O    | 0.59     | 1.97        | 1      | 1     |
| 1:A:30:ILE:HD13 | 1:A:30:ILE:O    | 0.58     | 1.99        | 12     | 1     |
| 1:A:26:VAL:HG13 | 1:A:26:VAL:O    | 0.56     | 2.00        | 4      | 2     |
| 1:A:36:GLY:O    | 1:A:39:ALA:HB3  | 0.56     | 2.00        | 11     | 6     |
| 1:A:20:TYR:CD2  | 1:A:21:LYS:N    | 0.55     | 2.74        | 2      | 1     |
| 1:A:53:VAL:HG12 | 1:A:53:VAL:O    | 0.55     | 2.02        | 7      | 2     |
| 1:A:26:VAL:HG13 | 1:A:27:PRO:HD2  | 0.55     | 1.79        | 18     | 2     |
| 1:A:44:TYR:CD1  | 1:A:44:TYR:C    | 0.54     | 2.85        | 9      | 2     |
| 1:A:67:MET:HE1  | 1:A:79:PRO:HB3  | 0.54     | 1.80        | 10     | 1     |
| 1:A:53:VAL:HG13 | 1:A:90:MET:HG2  | 0.54     | 1.80        | 5      | 1     |
| 1:A:43:ALA:HB2  | 1:A:55:VAL:HG11 | 0.54     | 1.79        | 1      | 1     |
| 1:A:44:TYR:O    | 1:A:46:VAL:HG23 | 0.54     | 2.03        | 10     | 1     |
| 1:A:92:LEU:O    | 1:A:95:VAL:HG22 | 0.53     | 2.03        | 19     | 1     |
| 1:A:25:GLY:O    | 1:A:26:VAL:CG2  | 0.53     | 2.57        | 12     | 2     |
| 1:A:62:PHE:CD2  | 1:A:66:ILE:CD1  | 0.52     | 2.93        | 9      | 1     |
| 1:A:62:PHE:C    | 1:A:66:ILE:HD12 | 0.52     | 2.29        | 9      | 1     |
| 1:A:59:THR:O    | 1:A:63:LEU:HD12 | 0.52     | 2.05        | 10     | 1     |
| 1:A:26:VAL:N    | 1:A:27:PRO:CD   | 0.51     | 2.73        | 12     | 3     |
| 1:A:45:ARG:C    | 1:A:46:VAL:CG2  | 0.51     | 2.80        | 19     | 1     |
| 1:A:25:GLY:O    | 1:A:26:VAL:CB   | 0.51     | 2.59        | 12     | 2     |
| 1:A:79:PRO:O    | 1:A:83:VAL:HG23 | 0.51     | 2.04        | 2      | 2     |
| 1:A:82:LEU:C    | 1:A:82:LEU:CD1  | 0.51     | 2.81        | 16     | 1     |
| 1:A:45:ARG:O    | 1:A:46:VAL:CG2  | 0.51     | 2.59        | 5      | 1     |
| 1:A:45:ARG:C    | 1:A:46:VAL:CG1  | 0.51     | 2.80        | 20     | 1     |
| 1:A:41:TYR:O    | 1:A:44:TYR:CB   | 0.51     | 2.60        | 17     | 3     |
| 1:A:27:PRO:O    | 1:A:28:SER:CB   | 0.51     | 2.59        | 20     | 2     |
| 1:A:39:ALA:O    | 1:A:43:ALA:CB   | 0.50     | 2.59        | 9      | 4     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:81:GLY:O    | 1:A:84:ALA:HB3  | 0.50     | 2.06        | 20     | 3     |
| 1:A:35:VAL:CG1  | 1:A:59:THR:OG1  | 0.50     | 2.60        | 10     | 1     |
| 1:A:13:THR:O    | 1:A:17:ILE:CG1  | 0.50     | 2.60        | 15     | 5     |
| 1:A:53:VAL:O    | 1:A:54:LYS:C    | 0.50     | 2.54        | 18     | 6     |
| 1:A:15:GLY:O    | 1:A:18:PHE:CB   | 0.50     | 2.60        | 13     | 6     |
| 1:A:37:CYS:O    | 1:A:41:TYR:CB   | 0.50     | 2.60        | 19     | 3     |
| 1:A:60:ALA:O    | 1:A:64:ALA:CB   | 0.50     | 2.60        | 16     | 2     |
| 1:A:11:LEU:C    | 1:A:11:LEU:HD13 | 0.49     | 2.32        | 4      | 1     |
| 1:A:11:LEU:C    | 1:A:11:LEU:CD1  | 0.49     | 2.85        | 4      | 1     |
| 1:A:55:VAL:HG23 | 1:A:56:SER:N    | 0.49     | 2.23        | 6      | 7     |
| 1:A:28:SER:OG   | 1:A:82:LEU:HD11 | 0.49     | 2.07        | 3      | 1     |
| 1:A:45:ARG:O    | 1:A:46:VAL:CB   | 0.49     | 2.61        | 5      | 2     |
| 1:A:37:CYS:O    | 1:A:38:LEU:C    | 0.49     | 2.56        | 12     | 15    |
| 1:A:86:LEU:C    | 1:A:86:LEU:CD1  | 0.48     | 2.86        | 1      | 1     |
| 1:A:26:VAL:HG23 | 1:A:26:VAL:O    | 0.48     | 2.08        | 17     | 2     |
| 1:A:25:GLY:C    | 1:A:26:VAL:CG2  | 0.48     | 2.86        | 19     | 1     |
| 1:A:12:VAL:O    | 1:A:16:SER:CB   | 0.48     | 2.61        | 9      | 2     |
| 1:A:95:VAL:C    | 1:A:97:LEU:N    | 0.48     | 2.70        | 14     | 5     |
| 1:A:35:VAL:HG13 | 1:A:36:GLY:N    | 0.48     | 2.23        | 7      | 3     |
| 1:A:22:ARG:O    | 1:A:23:ARG:CB   | 0.48     | 2.61        | 13     | 2     |
| 1:A:96:LEU:O    | 1:A:96:LEU:HD13 | 0.48     | 2.08        | 2      | 1     |
| 1:A:59:THR:O    | 1:A:63:LEU:CB   | 0.48     | 2.62        | 2      | 2     |
| 1:A:80:ALA:O    | 1:A:81:GLY:C    | 0.48     | 2.56        | 11     | 14    |
| 1:A:31:ALA:O    | 1:A:35:VAL:HG12 | 0.48     | 2.09        | 5      | 2     |
| 1:A:31:ALA:O    | 1:A:35:VAL:CG2  | 0.48     | 2.62        | 11     | 1     |
| 1:A:45:ARG:O    | 1:A:46:VAL:CG1  | 0.48     | 2.58        | 19     | 1     |
| 1:A:39:ALA:O    | 1:A:43:ALA:HB2  | 0.48     | 2.08        | 9      | 4     |
| 1:A:55:VAL:HG13 | 1:A:56:SER:N    | 0.48     | 2.24        | 14     | 2     |
| 1:A:30:ILE:HD13 | 1:A:30:ILE:C    | 0.48     | 2.34        | 12     | 1     |
| 1:A:42:GLY:O    | 1:A:46:VAL:HG22 | 0.47     | 2.09        | 9      | 2     |
| 1:A:63:LEU:O    | 1:A:66:ILE:CG1  | 0.47     | 2.62        | 11     | 1     |
| 1:A:45:ARG:O    | 1:A:46:VAL:HG12 | 0.47     | 2.08        | 20     | 1     |
| 1:A:14:PHE:CE1  | 1:A:18:PHE:CE1  | 0.47     | 3.02        | 5      | 1     |
| 1:A:10:ALA:O    | 1:A:14:PHE:CB   | 0.47     | 2.62        | 20     | 1     |
| 1:A:39:ALA:HB1  | 1:A:55:VAL:CG2  | 0.47     | 2.39        | 15     | 1     |
| 1:A:59:THR:CG2  | 1:A:60:ALA:N    | 0.47     | 2.77        | 17     | 1     |
| 1:A:19:GLY:O    | 1:A:20:TYR:C    | 0.47     | 2.58        | 14     | 5     |
| 1:A:25:GLY:O    | 1:A:26:VAL:C    | 0.47     | 2.58        | 17     | 4     |
| 1:A:11:LEU:HD13 | 1:A:11:LEU:O    | 0.47     | 2.09        | 4      | 1     |
| 1:A:46:VAL:HG23 | 1:A:47:SER:N    | 0.46     | 2.26        | 6      | 2     |
| 1:A:40:GLY:O    | 1:A:41:TYR:C    | 0.46     | 2.59        | 19     | 12    |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:15:GLY:O    | 1:A:16:SER:C    | 0.46     | 2.58        | 11     | 20    |
| 1:A:20:TYR:O    | 1:A:21:LYS:C    | 0.46     | 2.58        | 20     | 1     |
| 1:A:60:ALA:HB2  | 1:A:86:LEU:HD22 | 0.46     | 1.88        | 7      | 1     |
| 1:A:55:VAL:HG23 | 1:A:56:SER:H    | 0.46     | 1.71        | 11     | 4     |
| 1:A:39:ALA:O    | 1:A:40:GLY:C    | 0.46     | 2.58        | 19     | 3     |
| 1:A:64:ALA:O    | 1:A:67:MET:CG   | 0.46     | 2.64        | 7      | 1     |
| 1:A:61:PHE:O    | 1:A:65:THR:CB   | 0.46     | 2.63        | 11     | 1     |
| 1:A:62:PHE:O    | 1:A:66:ILE:CG1  | 0.46     | 2.64        | 19     | 1     |
| 1:A:13:THR:O    | 1:A:14:PHE:C    | 0.46     | 2.59        | 8      | 2     |
| 1:A:54:LYS:O    | 1:A:55:VAL:C    | 0.45     | 2.59        | 7      | 20    |
| 1:A:42:GLY:O    | 1:A:46:VAL:N    | 0.45     | 2.49        | 15     | 4     |
| 1:A:20:TYR:O    | 1:A:20:TYR:CD2  | 0.45     | 2.70        | 18     | 1     |
| 1:A:46:VAL:O    | 1:A:47:SER:C    | 0.45     | 2.60        | 12     | 3     |
| 1:A:96:LEU:O    | 1:A:97:LEU:C    | 0.45     | 2.59        | 14     | 14    |
| 1:A:30:ILE:C    | 1:A:30:ILE:CD1  | 0.45     | 2.89        | 12     | 1     |
| 1:A:30:ILE:CG2  | 1:A:31:ALA:N    | 0.45     | 2.78        | 17     | 2     |
| 1:A:46:VAL:C    | 1:A:47:SER:OG   | 0.45     | 2.59        | 19     | 1     |
| 1:A:61:PHE:C    | 1:A:61:PHE:CD1  | 0.45     | 2.94        | 15     | 2     |
| 1:A:19:GLY:C    | 1:A:21:LYS:N    | 0.45     | 2.74        | 14     | 1     |
| 1:A:22:ARG:O    | 1:A:23:ARG:C    | 0.45     | 2.60        | 20     | 2     |
| 1:A:91:ILE:HA   | 1:A:94:LEU:HD12 | 0.45     | 1.88        | 19     | 1     |
| 1:A:96:LEU:O    | 1:A:99:LEU:N    | 0.45     | 2.50        | 8      | 5     |
| 1:A:95:VAL:O    | 1:A:96:LEU:C    | 0.45     | 2.60        | 14     | 8     |
| 1:A:28:SER:CB   | 1:A:82:LEU:HD11 | 0.44     | 2.43        | 3      | 1     |
| 1:A:39:ALA:HB1  | 1:A:55:VAL:CG1  | 0.44     | 2.42        | 3      | 1     |
| 1:A:28:SER:O    | 1:A:29:LEU:C    | 0.44     | 2.60        | 20     | 20    |
| 1:A:9:ALA:O     | 1:A:13:THR:CB   | 0.44     | 2.65        | 9      | 2     |
| 1:A:35:VAL:O    | 1:A:36:GLY:C    | 0.44     | 2.60        | 16     | 2     |
| 1:A:98:LEU:O    | 1:A:99:LEU:C    | 0.44     | 2.61        | 9      | 5     |
| 1:A:60:ALA:HB2  | 1:A:86:LEU:HD11 | 0.44     | 1.88        | 5      | 1     |
| 1:A:53:VAL:O    | 1:A:53:VAL:CG2  | 0.44     | 2.60        | 12     | 1     |
| 1:A:47:SER:O    | 1:A:49:ASP:N    | 0.44     | 2.50        | 17     | 1     |
| 1:A:62:PHE:CE1  | 1:A:66:ILE:HD11 | 0.44     | 2.47        | 3      | 1     |
| 1:A:87:SER:O    | 1:A:88:LEU:C    | 0.44     | 2.59        | 12     | 6     |
| 1:A:35:VAL:CG1  | 1:A:59:THR:CG2  | 0.44     | 2.96        | 12     | 1     |
| 1:A:53:VAL:O    | 1:A:53:VAL:HG13 | 0.43     | 2.12        | 3      | 1     |
| 1:A:80:ALA:O    | 1:A:83:VAL:CG2  | 0.43     | 2.61        | 11     | 1     |
| 1:A:19:GLY:O    | 1:A:21:LYS:N    | 0.43     | 2.51        | 14     | 1     |
| 1:A:28:SER:O    | 1:A:31:ALA:HB3  | 0.43     | 2.14        | 4      | 1     |
| 1:A:44:TYR:C    | 1:A:47:SER:O    | 0.43     | 2.61        | 14     | 1     |
| 1:A:45:ARG:O    | 1:A:46:VAL:HG22 | 0.43     | 2.13        | 19     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:46:VAL:CG2  | 1:A:47:SER:N    | 0.43     | 2.82        | 6      | 1     |
| 1:A:35:VAL:CG1  | 1:A:59:THR:HG23 | 0.43     | 2.44        | 11     | 1     |
| 1:A:63:LEU:CD2  | 1:A:82:LEU:HD21 | 0.43     | 2.43        | 8      | 1     |
| 1:A:48:ASN:O    | 1:A:49:ASP:CB   | 0.43     | 2.65        | 19     | 1     |
| 1:A:43:ALA:O    | 1:A:46:VAL:O    | 0.43     | 2.36        | 17     | 1     |
| 1:A:33:LEU:O    | 1:A:37:CYS:CB   | 0.43     | 2.67        | 19     | 1     |
| 1:A:28:SER:OG   | 1:A:29:LEU:N    | 0.43     | 2.50        | 8      | 1     |
| 1:A:26:VAL:O    | 1:A:26:VAL:CG1  | 0.42     | 2.67        | 4      | 2     |
| 1:A:60:ALA:HB2  | 1:A:86:LEU:HG   | 0.42     | 1.91        | 10     | 1     |
| 1:A:79:PRO:O    | 1:A:80:ALA:C    | 0.42     | 2.62        | 14     | 3     |
| 1:A:14:PHE:O    | 1:A:17:ILE:HG22 | 0.42     | 2.14        | 19     | 2     |
| 1:A:13:THR:HG22 | 1:A:17:ILE:HD12 | 0.42     | 1.91        | 2      | 1     |
| 1:A:64:ALA:O    | 1:A:68:GLY:N    | 0.42     | 2.50        | 14     | 1     |
| 1:A:39:ALA:HB1  | 1:A:55:VAL:HG12 | 0.42     | 1.92        | 3      | 1     |
| 1:A:62:PHE:O    | 1:A:63:LEU:C    | 0.42     | 2.63        | 3      | 2     |
| 1:A:25:GLY:O    | 1:A:27:PRO:N    | 0.42     | 2.52        | 17     | 2     |
| 1:A:58:PHE:CD1  | 1:A:58:PHE:C    | 0.42     | 2.98        | 13     | 2     |
| 1:A:58:PHE:O    | 1:A:62:PHE:CB   | 0.42     | 2.67        | 8      | 1     |
| 1:A:44:TYR:O    | 1:A:47:SER:O    | 0.42     | 2.38        | 14     | 1     |
| 1:A:20:TYR:CG   | 1:A:21:LYS:N    | 0.42     | 2.88        | 2      | 1     |
| 1:A:46:VAL:O    | 1:A:47:SER:CB   | 0.42     | 2.68        | 3      | 2     |
| 1:A:57:LEU:O    | 1:A:61:PHE:CB   | 0.42     | 2.68        | 13     | 1     |
| 1:A:95:VAL:O    | 1:A:97:LEU:N    | 0.42     | 2.53        | 14     | 1     |
| 1:A:95:VAL:O    | 1:A:98:LEU:N    | 0.42     | 2.51        | 17     | 1     |
| 1:A:17:ILE:O    | 1:A:20:TYR:CD2  | 0.41     | 2.72        | 1      | 1     |
| 1:A:60:ALA:HB2  | 1:A:86:LEU:CD1  | 0.41     | 2.45        | 5      | 1     |
| 1:A:13:THR:O    | 1:A:17:ILE:HD12 | 0.41     | 2.15        | 12     | 1     |
| 1:A:26:VAL:N    | 1:A:27:PRO:HD2  | 0.41     | 2.31        | 12     | 2     |
| 1:A:26:VAL:HG22 | 1:A:26:VAL:O    | 0.41     | 2.14        | 7      | 1     |
| 1:A:83:VAL:HA   | 1:A:86:LEU:HD12 | 0.41     | 1.93        | 14     | 1     |
| 1:A:26:VAL:HG13 | 1:A:30:ILE:HG21 | 0.41     | 1.92        | 1      | 1     |
| 1:A:26:VAL:CG2  | 1:A:27:PRO:HD2  | 0.41     | 2.46        | 16     | 1     |
| 1:A:59:THR:HG22 | 1:A:60:ALA:N    | 0.41     | 2.31        | 17     | 1     |
| 1:A:55:VAL:HG13 | 1:A:56:SER:H    | 0.40     | 1.76        | 4      | 1     |
| 1:A:57:LEU:O    | 1:A:57:LEU:HD23 | 0.40     | 2.16        | 7      | 1     |
| 1:A:96:LEU:C    | 1:A:98:LEU:N    | 0.40     | 2.77        | 14     | 1     |
| 1:A:48:ASN:O    | 1:A:49:ASP:C    | 0.40     | 2.62        | 1      | 1     |
| 1:A:43:ALA:O    | 1:A:47:SER:O    | 0.40     | 2.38        | 14     | 1     |
| 1:A:46:VAL:O    | 1:A:48:ASN:N    | 0.40     | 2.55        | 18     | 1     |
| 1:A:17:ILE:O    | 1:A:21:LYS:O    | 0.40     | 2.39        | 20     | 1     |
| 1:A:42:GLY:O    | 1:A:46:VAL:HG12 | 0.40     | 2.17        | 13     | 1     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:A:19:GLY:O   | 1:A:20:TYR:O   | 0.40     | 2.40        | 15     | 1     |
| 1:A:26:VAL:CG1 | 1:A:27:PRO:HD2 | 0.40     | 2.46        | 18     | 1     |
| 1:A:90:MET:O   | 1:A:93:ARG:CB  | 0.40     | 2.70        | 20     | 1     |

## 6.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 79/108 (73%)    | 57±3 (72±4%) | 16±4 (20±5%) | 6±2 (8±2%) | <b>1</b>    | <b>14</b> |
| All | All   | 1580/2160 (73%) | 1136 (72%)   | 323 (20%)    | 121 (8%)   | <b>1</b>    | <b>14</b> |

All 23 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     | 20  | TYR  | 18             |
| 1   | A     | 28  | SER  | 10             |
| 1   | A     | 48  | ASN  | 9              |
| 1   | A     | 46  | VAL  | 8              |
| 1   | A     | 53  | VAL  | 8              |
| 1   | A     | 22  | ARG  | 8              |
| 1   | A     | 21  | LYS  | 7              |
| 1   | A     | 49  | ASP  | 6              |
| 1   | A     | 79  | PRO  | 6              |
| 1   | A     | 47  | SER  | 6              |
| 1   | A     | 25  | GLY  | 6              |
| 1   | A     | 23  | ARG  | 5              |
| 1   | A     | 26  | VAL  | 4              |
| 1   | A     | 24  | GLY  | 3              |
| 1   | A     | 15  | GLY  | 3              |
| 1   | A     | 40  | GLY  | 3              |
| 1   | A     | 27  | PRO  | 2              |
| 1   | A     | 39  | ALA  | 2              |
| 1   | A     | 13  | THR  | 2              |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 94  | LEU  | 2              |
| 1   | A     | 63  | LEU  | 1              |
| 1   | A     | 35  | VAL  | 1              |
| 1   | A     | 45  | ARG  | 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     | 59/85 (69%)     | 38±3 (64±6%) | 21±3 (36±6%) | 1           | 9 |
| All | All   | 1180/1700 (69%) | 754 (64%)    | 426 (36%)    | 1           | 9 |

All 48 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     | 88  | LEU  | 17             |
| 1   | A     | 11  | LEU  | 16             |
| 1   | A     | 98  | LEU  | 16             |
| 1   | A     | 96  | LEU  | 16             |
| 1   | A     | 63  | LEU  | 15             |
| 1   | A     | 29  | LEU  | 14             |
| 1   | A     | 57  | LEU  | 14             |
| 1   | A     | 67  | MET  | 14             |
| 1   | A     | 89  | MET  | 14             |
| 1   | A     | 94  | LEU  | 14             |
| 1   | A     | 82  | LEU  | 13             |
| 1   | A     | 92  | LEU  | 13             |
| 1   | A     | 97  | LEU  | 13             |
| 1   | A     | 38  | LEU  | 13             |
| 1   | A     | 21  | LYS  | 12             |
| 1   | A     | 22  | ARG  | 12             |
| 1   | A     | 23  | ARG  | 12             |
| 1   | A     | 33  | LEU  | 12             |
| 1   | A     | 54  | LYS  | 12             |
| 1   | A     | 90  | MET  | 12             |
| 1   | A     | 45  | ARG  | 12             |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 99  | LEU  | 12             |
| 1   | A     | 87  | SER  | 11             |
| 1   | A     | 16  | SER  | 10             |
| 1   | A     | 47  | SER  | 9              |
| 1   | A     | 56  | SER  | 9              |
| 1   | A     | 28  | SER  | 8              |
| 1   | A     | 93  | ARG  | 8              |
| 1   | A     | 49  | ASP  | 6              |
| 1   | A     | 66  | ILE  | 6              |
| 1   | A     | 86  | LEU  | 6              |
| 1   | A     | 20  | TYR  | 6              |
| 1   | A     | 30  | ILE  | 5              |
| 1   | A     | 48  | ASN  | 5              |
| 1   | A     | 14  | PHE  | 5              |
| 1   | A     | 37  | CYS  | 5              |
| 1   | A     | 46  | VAL  | 4              |
| 1   | A     | 41  | TYR  | 4              |
| 1   | A     | 26  | VAL  | 4              |
| 1   | A     | 17  | ILE  | 3              |
| 1   | A     | 65  | THR  | 3              |
| 1   | A     | 44  | TYR  | 2              |
| 1   | A     | 59  | THR  | 2              |
| 1   | A     | 55  | VAL  | 2              |
| 1   | A     | 18  | PHE  | 2              |
| 1   | A     | 34  | PHE  | 1              |
| 1   | A     | 91  | ILE  | 1              |
| 1   | A     | 8   | TYR  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 59% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 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                  | 819 |
| Number of shifts mapped to atoms        | 819 |
| 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           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 98       | $0.05 \pm 0.16$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 83       | $0.64 \pm 0.06$                 | Should be checked          |
| $^{13}\text{C}'$       | 81       | $2.19 \pm 0.11$                 | Should be applied          |
| $^{15}\text{N}$        | 96       | $0.12 \pm 0.24$                 | 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 64%, i.e. 693 atoms were assigned a chemical shift out of a possible 1090. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 400/408 (98%) | 168/170 (99%) | 154/160 (96%)   | 78/78 (100%)    |
| Sidechain | 285/586 (49%) | 142/397 (36%) | 142/174 (82%)   | 1/15 (7%)       |

*Continued on next page...*

Continued from previous page...

|          | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 8/96 (8%)      | 8/46 (17%)     | 0/50 (0%)       | 0/0 (—%)        |
| Overall  | 693/1090 (64%) | 318/613 (52%)  | 296/384 (77%)   | 79/93 (85%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 59%, i.e. 819 atoms were assigned a chemical shift out of a possible 1398. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 472/504 (94%)  | 197/209 (94%)  | 179/198 (90%)   | 96/97 (99%)     |
| Sidechain | 339/778 (44%)  | 167/520 (32%)  | 171/230 (74%)   | 1/28 (4%)       |
| Aromatic  | 8/116 (7%)     | 8/56 (14%)     | 0/60 (0%)       | 0/0 (—%)        |
| Overall   | 819/1398 (59%) | 372/785 (47%)  | 350/488 (72%)   | 97/125 (78%)    |

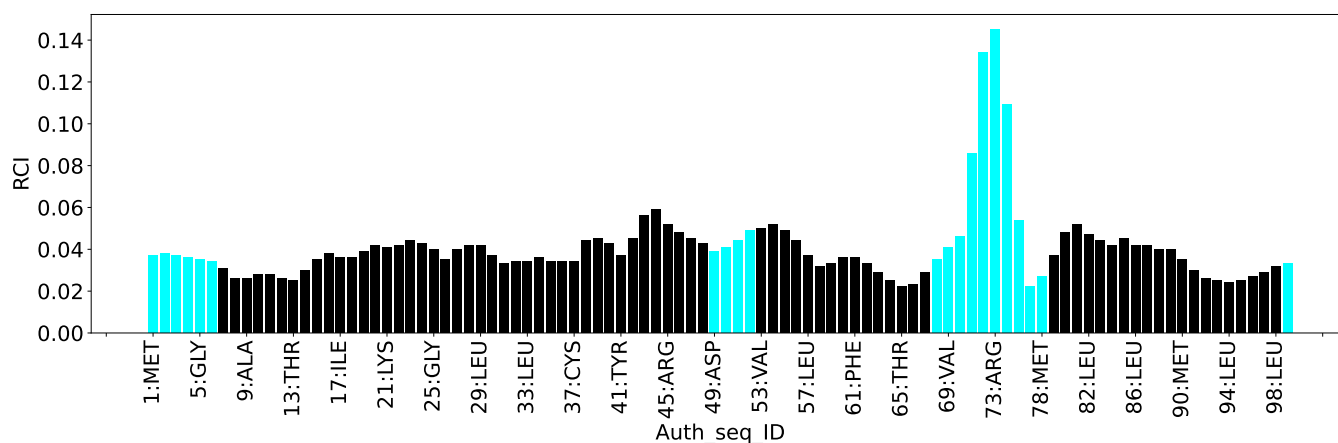
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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                                | 1001  |
| Intra-residue ( $ i-j =0$ )                              | 0     |
| Sequential ( $ i-j =1$ )                                 | 8     |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 70    |
| Long range ( $ i-j \geq 5$ )                             | 791   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 132   |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 9.3   |
| Number of long range restraints per residue <sup>1</sup> | 7.3   |

<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)  | 15.4                                   | 0.2     |
| 0.2-0.5 (Medium) | 33.0                                   | 0.5     |
| >0.5 (Large)     | 464.2                                  | 31.83   |

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

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis ⓘ

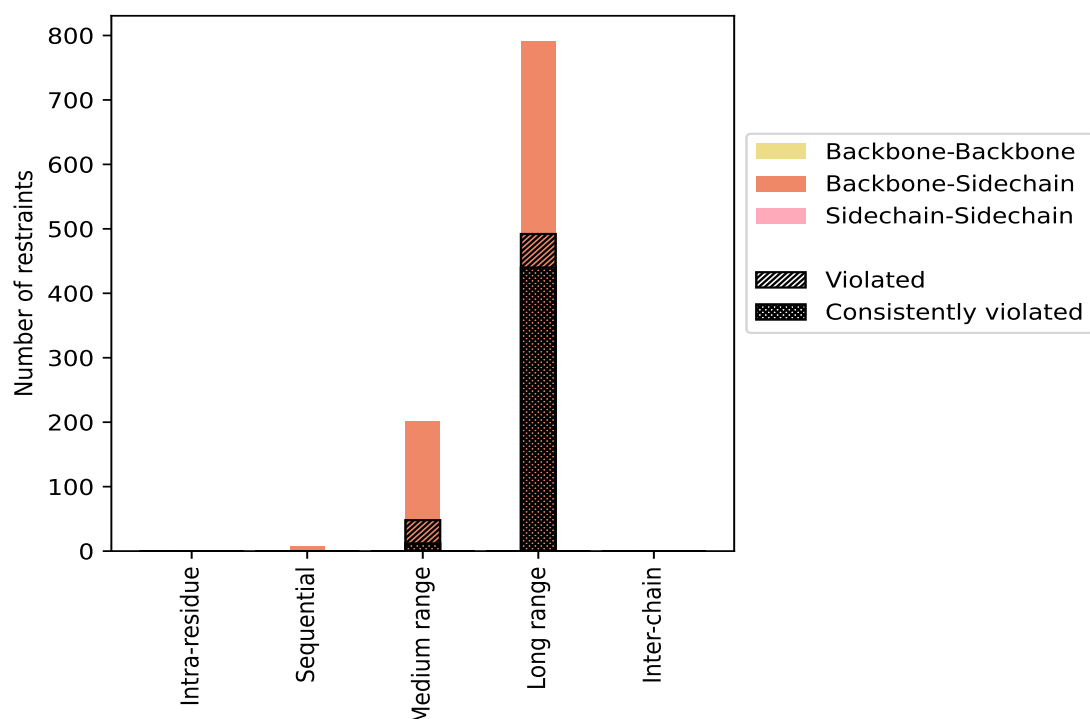
### 9.1 Summary of distance violations ⓘ

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> |
| Intra-residue ( $ i-j =0$ )            | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| 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            |
| Sequential ( $ i-j =1$ )               | 8     | 0.8            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 8     | 0.8            | 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            |
| Medium range ( $ i-j >1$ & $ i-j <5$ ) | 70    | 7.0            | 2                     | 2.9            | 0.2            | 1                                  | 1.4            | 0.1            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 70    | 7.0            | 2                     | 2.9            | 0.2            | 1                                  | 1.4            | 0.1            |
| Sidechain-Sidechain                    | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Long range ( $ i-j \geq 5$ )           | 791   | 79.0           | 492                   | 62.2           | 49.2           | 440                                | 55.6           | 44.0           |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 791   | 79.0           | 492                   | 62.2           | 49.2           | 440                                | 55.6           | 44.0           |
| Sidechain-Sidechain                    | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Inter-chain                            | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| 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            |
| Hydrogen bond                          | 132   | 13.2           | 46                    | 34.8           | 4.6            | 11                                 | 8.3            | 1.1            |
| Disulfide bond                         | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total                                  | 1001  | 100.0          | 540                   | 53.9           | 53.9           | 452                                | 45.2           | 45.2           |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 1001  | 100.0          | 540                   | 53.9           | 53.9           | 452                                | 45.2           | 45.2           |
| Sidechain-Sidechain                    | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |

<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 disulfied 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        | 0                    | 0               | 35              | 481             | 0               | 516   | 4.8      | 27.53   | 4.14                | 3.88       |
| 2        | 0                    | 0               | 29              | 482             | 0               | 511   | 5.0      | 27.95   | 4.45                | 3.91       |
| 3        | 0                    | 0               | 35              | 477             | 0               | 512   | 4.74     | 25.36   | 4.06                | 3.87       |
| 4        | 0                    | 0               | 36              | 481             | 0               | 517   | 4.58     | 23.98   | 3.88                | 3.63       |
| 5        | 0                    | 0               | 29              | 475             | 0               | 504   | 4.55     | 24.55   | 3.7                 | 3.88       |
| 6        | 0                    | 0               | 37              | 479             | 0               | 516   | 4.97     | 30.62   | 4.43                | 3.97       |
| 7        | 0                    | 0               | 36              | 481             | 0               | 517   | 5.05     | 28.73   | 4.52                | 4.04       |
| 8        | 0                    | 0               | 38              | 479             | 0               | 517   | 5.02     | 29.36   | 4.49                | 4.03       |
| 9        | 0                    | 0               | 30              | 480             | 0               | 510   | 5.12     | 31.83   | 4.61                | 4.19       |
| 10       | 0                    | 0               | 39              | 480             | 0               | 519   | 4.84     | 28.07   | 4.32                | 3.89       |

*Continued on next page...*

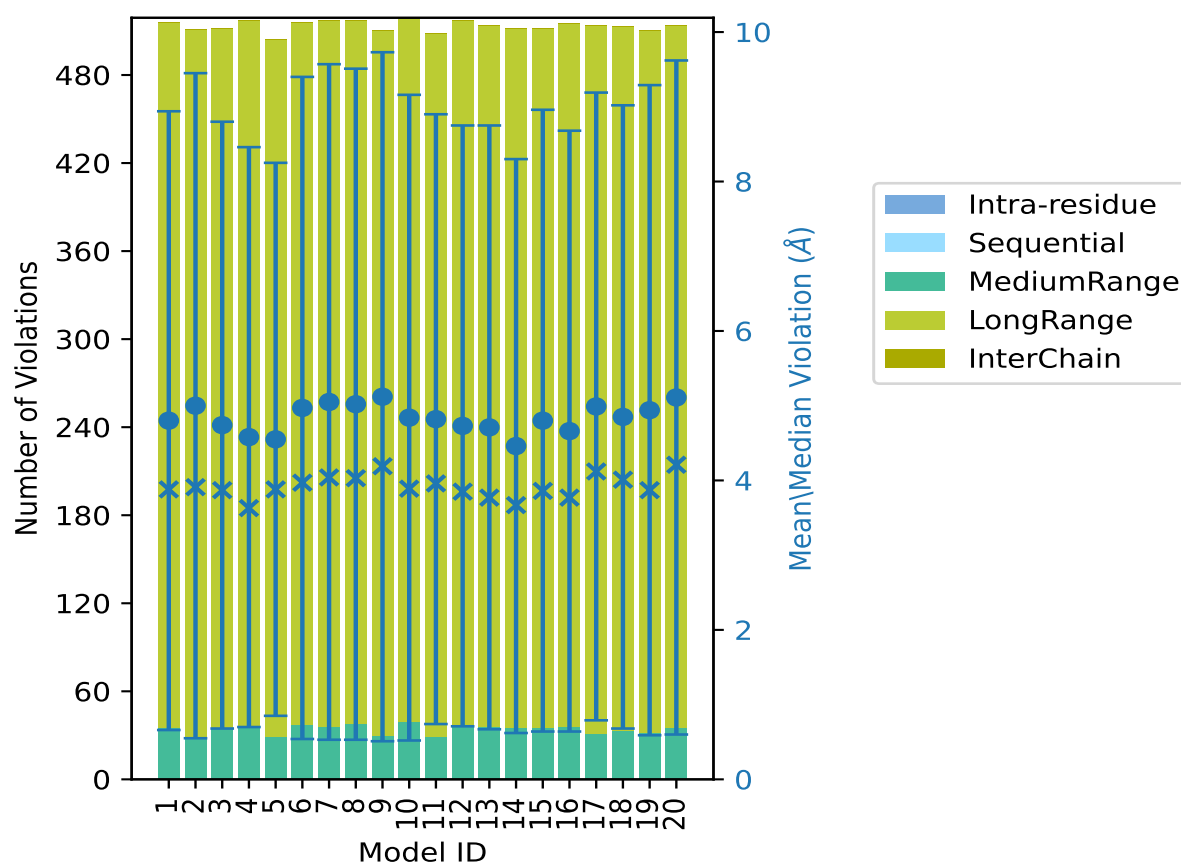
Continued from previous page...

| 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       | 0                    | 0               | 29              | 479             | 0               | 508   | 4.82     | 26.15   | 4.08                | 3.96       |
| 12       | 0                    | 0               | 36              | 481             | 0               | 517   | 4.73     | 25.35   | 4.02                | 3.85       |
| 13       | 0                    | 0               | 36              | 478             | 0               | 514   | 4.71     | 28.94   | 4.04                | 3.77       |
| 14       | 0                    | 0               | 35              | 477             | 0               | 512   | 4.46     | 25.21   | 3.84                | 3.67       |
| 15       | 0                    | 0               | 35              | 477             | 0               | 512   | 4.8      | 26.48   | 4.16                | 3.86       |
| 16       | 0                    | 0               | 36              | 479             | 0               | 515   | 4.66     | 24.08   | 4.02                | 3.77       |
| 17       | 0                    | 0               | 31              | 483             | 0               | 514   | 4.99     | 26.99   | 4.2                 | 4.12       |
| 18       | 0                    | 0               | 33              | 480             | 0               | 513   | 4.85     | 28.53   | 4.17                | 4.01       |
| 19       | 0                    | 0               | 32              | 478             | 0               | 510   | 4.94     | 29.99   | 4.35                | 3.87       |
| 20       | 0                    | 0               | 35              | 479             | 0               | 514   | 5.11     | 30.02   | 4.51                | 4.21       |

<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

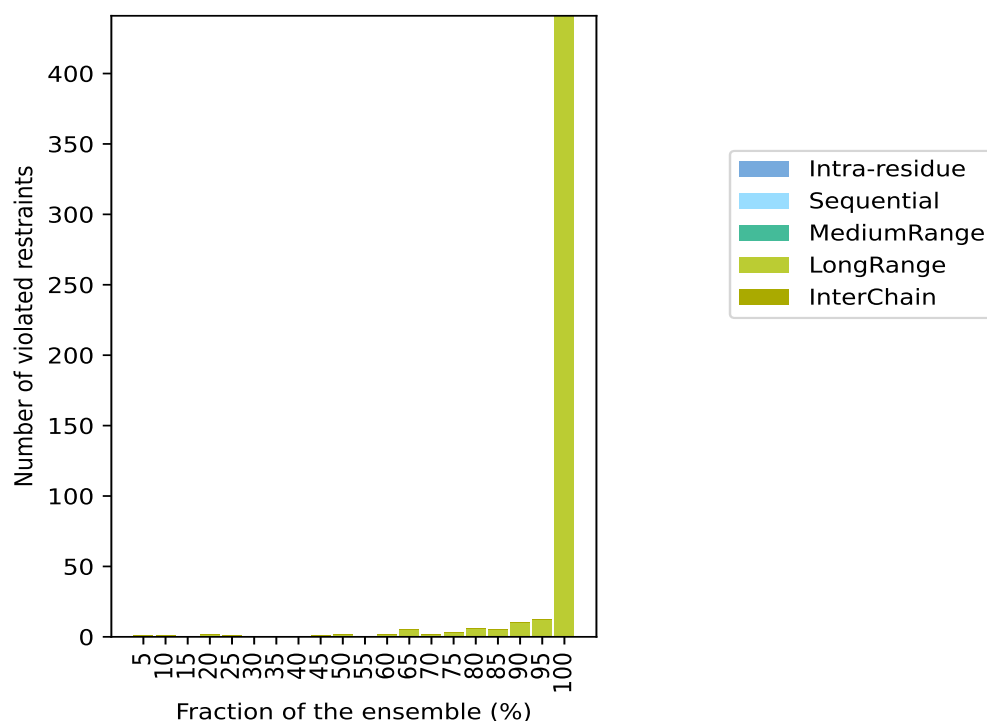
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 375(IR:0, SQ:8, MR:68, LR:299, IC:0) restraints are not violated 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>       | %     |
| 0                             | 0               | 0               | 1               | 0               | 1     | 1                        | 5.0   |
| 0                             | 0               | 0               | 1               | 0               | 1     | 2                        | 10.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 3                        | 15.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 4                        | 20.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 5                        | 25.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 6                        | 30.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 7                        | 35.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 8                        | 40.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 9                        | 45.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 10                       | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 55.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 12                       | 60.0  |
| 0                             | 0               | 0               | 5               | 0               | 5     | 13                       | 65.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 14                       | 70.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 15                       | 75.0  |
| 0                             | 0               | 0               | 6               | 0               | 6     | 16                       | 80.0  |
| 0                             | 0               | 0               | 5               | 0               | 5     | 17                       | 85.0  |
| 0                             | 0               | 0               | 10              | 0               | 10    | 18                       | 90.0  |
| 0                             | 0               | 0               | 12              | 0               | 12    | 19                       | 95.0  |
| 0                             | 0               | 1               | 440             | 0               | 441   | 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

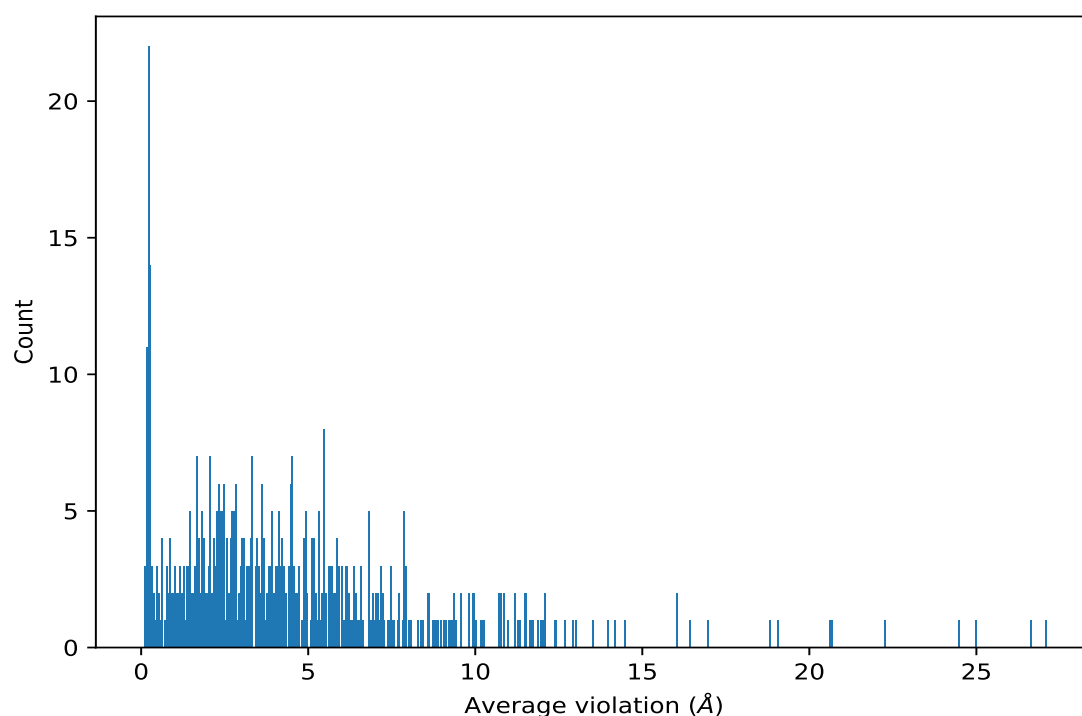
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|---------|--------------|---------------|---------------------|----------|---------------------|------------|
| (1,339) | 1:2:A:ASP:H  | 1:47:A:SER:CB | 20                  | 27.07    | 2.52                | 27.35      |
| (1,345) | 1:3:A:LEU:H  | 1:47:A:SER:CB | 20                  | 26.63    | 2.8                 | 27.01      |
| (1,352) | 1:4:A:ILE:H  | 1:47:A:SER:CB | 20                  | 24.99    | 1.99                | 24.86      |
| (1,359) | 1:5:A:GLY:H  | 1:47:A:SER:CB | 20                  | 24.45    | 1.82                | 24.86      |
| (1,366) | 1:6:A:PHE:H  | 1:47:A:SER:CB | 20                  | 22.28    | 1.27                | 22.52      |
| (1,373) | 1:7:A:GLY:H  | 1:47:A:SER:CB | 20                  | 20.68    | 1.21                | 20.76      |
| (1,380) | 1:8:A:TYR:H  | 1:47:A:SER:CB | 20                  | 20.61    | 1.03                | 20.76      |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 20                  | 19.09    | 1.11                | 19.1       |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 20                  | 18.8     | 2.12                | 19.37      |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 20                  | 16.95    | 0.99                | 17.11      |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 20                  | 16.42    | 0.94                | 16.52      |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 20                  | 16.03    | 0.82                | 16.06      |
| (1,346) | 1:3:A:LEU:H  | 1:56:A:SER:CB | 20                  | 16.01    | 3.77                | 15.92      |
| (1,340) | 1:2:A:ASP:H  | 1:56:A:SER:CB | 20                  | 14.47    | 3.69                | 14.4       |
| (1,353) | 1:4:A:ILE:H  | 1:56:A:SER:CB | 20                  | 14.15    | 2.67                | 13.46      |
| (1,413) | 1:13:A:THR:H | 1:47:A:SER:CB | 20                  | 13.98    | 0.85                | 14.0       |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 20                  | 13.52    | 3.76                | 14.75      |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 20                  | 13.01    | 2.33                | 13.12      |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 20                  | 12.92    | 3.04                | 13.77      |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 20                  | 12.67    | 2.59                | 12.95      |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 20                  | 12.41    | 1.02                | 12.5       |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 20                  | 12.35    | 2.39                | 12.74      |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 20                  | 12.09    | 0.88                | 12.24      |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 20                  | 12.07    | 1.35                | 11.99      |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 20                  | 12.02    | 2.56                | 11.48      |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 20                  | 11.97    | 0.91                | 11.94      |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 20                  | 11.88    | 1.38                | 11.54      |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 20                  | 11.74    | 2.78                | 11.38      |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 20                  | 11.64    | 0.75                | 11.49      |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 20                  | 11.5     | 0.65                | 11.31      |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 20                  | 11.5     | 1.94                | 11.46      |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 20                  | 11.49    | 3.59                | 10.76      |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 20                  | 11.46    | 2.26                | 12.24      |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 20                  | 11.32    | 1.0                 | 11.08      |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 20                  | 11.27    | 1.86                | 11.27      |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 20                  | 11.16    | 2.04                | 11.64      |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 20                  | 11.16    | 2.71                | 11.98      |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 20                  | 10.97    | 1.43                | 10.8       |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 20                  | 10.86    | 1.71                | 10.44      |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 20                  | 10.85    | 1.43                | 11.2       |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 20                  | 10.79    | 1.02                | 10.96      |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 20                  | 10.77    | 2.39                | 10.89      |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 20                  | 10.71    | 1.17                | 10.29      |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 20                  | 10.71    | 0.16                | 10.73      |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 20                  | 10.28    | 1.3                 | 10.26      |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 20                  | 10.23    | 1.71                | 10.62      |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 20                  | 10.19    | 1.39                | 10.62      |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 20                  | 10.04    | 2.03                | 9.72       |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 20                  | 9.99     | 1.61                | 10.0       |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 20                  | 9.95     | 2.16                | 9.62       |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 20                  | 9.94     | 0.19                | 9.95       |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 20                  | 9.9      | 1.49                | 10.05      |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 20                  | 9.84     | 1.16                | 9.99       |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 20                  | 9.59     | 4.3                 | 8.95       |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 20                  | 9.58     | 1.32                | 9.52       |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 20                  | 9.42     | 2.62                | 10.12      |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 20                  | 9.38     | 1.06                | 9.68       |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 20                  | 9.37     | 2.61                | 9.8        |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 20                  | 9.34     | 1.64                | 9.48       |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 20                  | 9.26     | 0.67                | 9.15       |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 20                  | 9.24     | 1.6                 | 9.08       |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 20                  | 9.13     | 1.85                | 8.96       |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 20                  | 9.07     | 1.57                | 9.27       |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 20                  | 8.98     | 0.06                | 9.0        |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 20                  | 8.88     | 1.74                | 9.05       |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 20                  | 8.83     | 2.28                | 8.64       |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 20                  | 8.78     | 4.49                | 8.18       |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 20                  | 8.7      | 0.99                | 8.68       |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 20                  | 8.63     | 0.51                | 8.68       |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 20                  | 8.6      | 0.72                | 8.52       |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 20                  | 8.58     | 0.93                | 8.66       |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 20                  | 8.55     | 1.42                | 8.59       |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 20                  | 8.44     | 1.67                | 8.6        |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 20                  | 8.35     | 1.54                | 8.65       |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 20                  | 8.27     | 2.16                | 8.88       |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 20                  | 8.05     | 1.13                | 8.41       |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 20                  | 8.0      | 1.15                | 8.04       |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 20                  | 7.92     | 0.97                | 7.96       |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 20                  | 7.92     | 3.01                | 7.02       |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 20                  | 7.91     | 1.01                | 7.76       |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 20                  | 7.89     | 1.83                | 8.15       |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 20                  | 7.87     | 1.27                | 7.69       |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 20                  | 7.87     | 1.3                 | 7.61       |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 20                  | 7.86     | 0.28                | 8.0        |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 20                  | 7.85     | 1.54                | 8.15       |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 20                  | 7.8      | 0.71                | 7.52       |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 20                  | 7.7      | 0.35                | 7.89       |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 20                  | 7.7      | 1.63                | 7.9        |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 20                  | 7.67     | 1.66                | 7.54       |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 20                  | 7.55     | 0.99                | 7.23       |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 20                  | 7.54     | 0.28                | 7.54       |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 20                  | 7.47     | 0.36                | 7.52       |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 20                  | 7.47     | 0.51                | 7.48       |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 20                  | 7.46     | 0.39                | 7.49       |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 20                  | 7.43     | 0.24                | 7.49       |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 20                  | 7.38     | 0.49                | 7.42       |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 20                  | 7.25     | 1.24                | 7.02       |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 20                  | 7.24     | 0.59                | 7.08       |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 20                  | 7.24     | 0.64                | 7.26       |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 20                  | 7.19     | 1.09                | 7.3        |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 20                  | 7.17     | 1.14                | 7.3        |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 20                  | 7.15     | 0.71                | 7.32       |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 20                  | 7.14     | 0.76                | 7.02       |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 20                  | 7.09     | 0.57                | 7.16       |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 20                  | 7.05     | 0.48                | 6.96       |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 20                  | 7.0      | 0.9                 | 7.02       |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 20                  | 7.0      | 0.38                | 7.08       |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 20                  | 6.99     | 0.68                | 7.11       |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 20                  | 6.93     | 0.12                | 6.93       |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 20                  | 6.92     | 0.38                | 6.96       |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 20                  | 6.89     | 0.54                | 7.06       |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 20                  | 6.83     | 0.41                | 6.84       |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 20                  | 6.82     | 1.05                | 6.78       |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 20                  | 6.81     | 0.48                | 6.69       |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 20                  | 6.8      | 0.77                | 6.75       |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 20                  | 6.8      | 1.07                | 6.84       |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 20                  | 6.62     | 2.26                | 6.39       |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 20                  | 6.57     | 0.91                | 6.46       |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 20                  | 6.57     | 0.97                | 6.89       |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 20                  | 6.57     | 0.33                | 6.62       |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 20                  | 6.54     | 0.52                | 6.48       |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 20                  | 6.49     | 0.41                | 6.46       |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 20                  | 6.44     | 0.9                 | 6.4        |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 20                  | 6.42     | 1.54                | 5.96       |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 20                  | 6.37     | 0.39                | 6.34       |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 20                  | 6.36     | 0.54                | 6.48       |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 20                  | 6.35     | 0.42                | 6.24       |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 20                  | 6.32     | 0.68                | 6.32       |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 20                  | 6.26     | 0.34                | 6.29       |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 20                  | 6.24     | 1.55                | 5.99       |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 20                  | 6.22     | 0.37                | 6.21       |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 20                  | 6.18     | 1.17                | 6.54       |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 20                  | 6.17     | 1.32                | 6.68       |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 20                  | 6.16     | 0.2                 | 6.28       |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 20                  | 6.12     | 1.04                | 6.36       |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 20                  | 6.11     | 1.21                | 6.24       |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 20                  | 6.1      | 0.72                | 6.19       |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 20                  | 6.08     | 0.92                | 6.44       |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 20                  | 6.02     | 0.49                | 6.28       |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 20                  | 6.0      | 0.71                | 6.03       |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 20                  | 6.0      | 1.36                | 6.22       |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 20                  | 5.94     | 0.09                | 5.98       |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 20                  | 5.92     | 0.75                | 5.96       |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 20                  | 5.9      | 0.12                | 5.91       |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 20                  | 5.87     | 0.51                | 5.81       |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 20                  | 5.86     | 0.54                | 5.98       |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 20                  | 5.86     | 0.94                | 5.96       |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 20                  | 5.85     | 0.51                | 5.74       |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 20                  | 5.84     | 1.26                | 6.1        |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 20                  | 5.83     | 0.15                | 5.9        |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 20                  | 5.79     | 1.77                | 5.98       |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 20                  | 5.78     | 0.45                | 5.95       |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 20                  | 5.74     | 0.45                | 5.77       |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 20                  | 5.71     | 1.19                | 5.65       |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 20                  | 5.71     | 0.3                 | 5.68       |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 20                  | 5.69     | 0.66                | 5.69       |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 20                  | 5.65     | 0.56                | 5.96       |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 20                  | 5.65     | 2.3                 | 6.16       |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 20                  | 5.64     | 1.88                | 5.66       |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 20                  | 5.62     | 0.35                | 5.66       |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 20                  | 5.6      | 0.17                | 5.6        |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 20                  | 5.54     | 0.58                | 5.58       |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 20                  | 5.52     | 1.59                | 5.78       |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 20                  | 5.49     | 0.42                | 5.69       |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 20                  | 5.48     | 0.66                | 5.7        |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 20                  | 5.48     | 0.19                | 5.48       |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 20                  | 5.47     | 0.33                | 5.47       |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 20                  | 5.47     | 0.86                | 5.9        |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 20                  | 5.46     | 0.2                 | 5.46       |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 20                  | 5.46     | 0.85                | 5.6        |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 20                  | 5.45     | 0.54                | 5.56       |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 20                  | 5.41     | 0.17                | 5.38       |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 20                  | 5.41     | 0.4                 | 5.35       |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 20                  | 5.39     | 0.93                | 5.16       |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 20                  | 5.34     | 0.16                | 5.36       |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 20                  | 5.34     | 1.17                | 5.42       |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 20                  | 5.33     | 0.94                | 5.43       |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 20                  | 5.32     | 0.69                | 5.26       |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 20                  | 5.32     | 0.75                | 5.36       |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 20                  | 5.29     | 1.08                | 5.13       |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 20                  | 5.22     | 0.46                | 5.18       |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 20                  | 5.2      | 0.38                | 5.14       |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 20                  | 5.18     | 0.74                | 5.2        |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 20                  | 5.17     | 0.18                | 5.15       |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 20                  | 5.16     | 0.52                | 5.2        |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 20                  | 5.15     | 1.3                 | 5.22       |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 20                  | 5.14     | 0.79                | 5.48       |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 20                  | 5.11     | 0.89                | 5.43       |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 20                  | 5.11     | 0.6                 | 5.2        |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 20                  | 5.1      | 1.57                | 5.64       |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 20                  | 5.09     | 0.93                | 5.31       |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 20                  | 4.99     | 0.95                | 5.26       |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 20                  | 4.97     | 0.43                | 4.97       |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 20                  | 4.93     | 0.57                | 4.84       |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 20                  | 4.92     | 0.17                | 4.88       |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 20                  | 4.92     | 0.76                | 5.08       |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 20                  | 4.92     | 0.56                | 4.97       |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 20                  | 4.91     | 0.44                | 5.02       |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 20                  | 4.89     | 0.31                | 4.82       |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 20                  | 4.89     | 0.64                | 5.12       |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 20                  | 4.88     | 0.16                | 4.85       |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 20                  | 4.86     | 1.49                | 4.34       |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 20                  | 4.84     | 0.73                | 5.11       |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 20                  | 4.74     | 0.29                | 4.78       |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 20                  | 4.72     | 1.04                | 4.9        |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 20                  | 4.7      | 0.28                | 4.66       |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 20                  | 4.69     | 0.96                | 4.76       |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 20                  | 4.66     | 1.49                | 4.54       |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 20                  | 4.63     | 0.54                | 4.8        |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 20                  | 4.63     | 3.36                | 3.17       |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 20                  | 4.59     | 0.36                | 4.61       |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 20                  | 4.59     | 0.39                | 4.66       |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 20                  | 4.55     | 0.49                | 4.62       |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 20                  | 4.53     | 0.22                | 4.58       |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 20                  | 4.51     | 0.49                | 4.54       |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 20                  | 4.51     | 0.99                | 4.64       |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 20                  | 4.51     | 0.47                | 4.4        |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 20                  | 4.51     | 1.45                | 5.01       |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 20                  | 4.5      | 0.45                | 4.54       |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 20                  | 4.5      | 0.56                | 4.39       |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 20                  | 4.49     | 0.38                | 4.59       |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 20                  | 4.49     | 1.08                | 4.36       |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 20                  | 4.47     | 0.4                 | 4.5        |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 20                  | 4.47     | 0.66                | 4.57       |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 20                  | 4.46     | 0.58                | 4.47       |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 20                  | 4.45     | 0.72                | 4.4        |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 20                  | 4.43     | 1.5                 | 4.67       |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 20                  | 4.41     | 0.88                | 4.58       |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 20                  | 4.4      | 0.6                 | 4.56       |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 20                  | 4.34     | 0.46                | 4.37       |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 20                  | 4.3      | 0.34                | 4.31       |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 20                  | 4.26     | 0.41                | 4.32       |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 20                  | 4.25     | 0.66                | 4.29       |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 20                  | 4.25     | 0.44                | 4.34       |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 20                  | 4.24     | 0.84                | 4.2        |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 20                  | 4.23     | 1.13                | 4.27       |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 20                  | 4.22     | 1.59                | 4.42       |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 20                  | 4.2      | 0.55                | 4.39       |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 20                  | 4.19     | 0.97                | 3.92       |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 20                  | 4.17     | 1.12                | 4.24       |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 20                  | 4.16     | 0.29                | 4.18       |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 20                  | 4.13     | 1.34                | 3.8        |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 20                  | 4.12     | 1.18                | 3.92       |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 20                  | 4.11     | 1.12                | 3.94       |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 20                  | 4.11     | 0.22                | 4.12       |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 20                  | 4.1      | 0.25                | 4.19       |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 20                  | 4.06     | 0.76                | 3.95       |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 20                  | 4.06     | 0.69                | 4.38       |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 20                  | 4.06     | 0.38                | 4.14       |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 20                  | 4.02     | 0.86                | 3.96       |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 20                  | 4.0      | 0.35                | 4.0        |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 20                  | 4.0      | 0.29                | 4.02       |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 20                  | 3.98     | 0.99                | 3.77       |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 20                  | 3.96     | 0.71                | 3.76       |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 20                  | 3.92     | 0.59                | 3.84       |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 20                  | 3.92     | 0.8                 | 3.94       |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 20                  | 3.91     | 0.36                | 3.9        |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 20                  | 3.91     | 0.5                 | 3.78       |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 20                  | 3.91     | 1.85                | 3.58       |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 20                  | 3.89     | 0.61                | 3.77       |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 20                  | 3.85     | 0.98                | 4.09       |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 20                  | 3.85     | 0.57                | 4.04       |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 20                  | 3.82     | 0.74                | 3.85       |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 20                  | 3.81     | 1.23                | 3.6        |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 20                  | 3.81     | 0.85                | 4.19       |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 20                  | 3.78     | 0.97                | 3.96       |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 20                  | 3.76     | 1.01                | 3.92       |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 20                  | 3.72     | 1.1                 | 3.7        |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 20                  | 3.69     | 0.36                | 3.76       |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 20                  | 3.68     | 0.77                | 3.6        |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 20                  | 3.68     | 0.33                | 3.71       |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 20                  | 3.64     | 1.13                | 3.63       |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 20                  | 3.64     | 0.1                 | 3.6        |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 20                  | 3.62     | 0.44                | 3.62       |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 20                  | 3.62     | 0.27                | 3.58       |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 20                  | 3.6      | 0.51                | 3.64       |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 20                  | 3.6      | 1.16                | 3.6        |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 20                  | 3.58     | 0.67                | 3.55       |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 20                  | 3.57     | 1.29                | 3.43       |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 20                  | 3.53     | 0.22                | 3.5        |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 20                  | 3.53     | 0.56                | 3.27       |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 20                  | 3.51     | 0.11                | 3.49       |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 20                  | 3.49     | 1.15                | 3.37       |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 20                  | 3.46     | 0.41                | 3.43       |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 20                  | 3.46     | 0.95                | 3.26       |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 20                  | 3.46     | 0.36                | 3.62       |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 20                  | 3.42     | 1.44                | 3.19       |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 20                  | 3.41     | 0.43                | 3.29       |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 20                  | 3.33     | 1.45                | 3.5        |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 20                  | 3.32     | 0.74                | 3.25       |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 20                  | 3.31     | 1.2                 | 3.28       |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 20                  | 3.3      | 0.78                | 3.53       |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 20                  | 3.3      | 0.44                | 3.26       |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 20                  | 3.29     | 1.13                | 3.18       |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 20                  | 3.26     | 0.5                 | 3.3        |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 20                  | 3.25     | 0.27                | 3.2        |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 20                  | 3.25     | 0.35                | 3.17       |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 20                  | 3.23     | 1.01                | 3.28       |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 20                  | 3.23     | 1.62                | 2.72       |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 20                  | 3.23     | 0.48                | 3.26       |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 20                  | 3.17     | 1.59                | 2.82       |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 20                  | 3.17     | 0.34                | 3.22       |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 20                  | 3.16     | 0.11                | 3.12       |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 20                  | 3.1      | 0.26                | 3.1        |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 20                  | 3.09     | 0.33                | 3.08       |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 20                  | 3.07     | 0.56                | 2.95       |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 20                  | 3.05     | 0.65                | 2.99       |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 20                  | 3.05     | 0.47                | 3.04       |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 20                  | 3.01     | 0.16                | 2.97       |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 20                  | 3.0      | 0.01                | 3.0        |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 20                  | 3.0      | 0.6                 | 2.94       |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 20                  | 3.0      | 0.24                | 3.0        |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 20                  | 2.97     | 0.41                | 3.09       |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 20                  | 2.95     | 0.32                | 2.96       |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 20                  | 2.9      | 0.54                | 2.94       |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 20                  | 2.86     | 0.47                | 2.76       |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 20                  | 2.84     | 0.6                 | 2.6        |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 20                  | 2.82     | 1.39                | 2.58       |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 20                  | 2.81     | 0.89                | 2.66       |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 20                  | 2.81     | 0.36                | 2.76       |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 20                  | 2.8      | 0.42                | 2.81       |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 20                  | 2.79     | 0.55                | 2.7        |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 20                  | 2.79     | 0.3                 | 2.88       |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 20                  | 2.77     | 0.12                | 2.78       |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 20                  | 2.76     | 0.98                | 2.99       |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 20                  | 2.75     | 1.35                | 2.73       |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 20                  | 2.73     | 0.82                | 2.66       |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 20                  | 2.72     | 1.31                | 2.89       |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 20                  | 2.72     | 0.98                | 2.82       |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 20                  | 2.72     | 0.85                | 2.54       |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 20                  | 2.7      | 0.36                | 2.64       |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 20                  | 2.69     | 0.28                | 2.74       |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 20                  | 2.67     | 0.37                | 2.78       |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 20                  | 2.65     | 0.96                | 2.5        |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 20                  | 2.65     | 0.97                | 2.56       |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 20                  | 2.63     | 0.58                | 2.56       |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 20                  | 2.61     | 1.11                | 2.53       |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 20                  | 2.57     | 0.67                | 2.44       |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 20                  | 2.56     | 1.03                | 2.65       |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 20                  | 2.55     | 0.79                | 2.5        |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 20                  | 2.55     | 0.29                | 2.58       |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 20                  | 2.5      | 1.62                | 1.98       |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 20                  | 2.48     | 1.18                | 2.34       |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 20                  | 2.48     | 0.21                | 2.49       |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 20                  | 2.47     | 0.51                | 2.56       |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 20                  | 2.45     | 0.31                | 2.46       |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 20                  | 2.44     | 0.55                | 2.41       |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 20                  | 2.44     | 0.36                | 2.45       |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 20                  | 2.44     | 0.6                 | 2.34       |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 20                  | 2.42     | 1.08                | 2.28       |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 20                  | 2.42     | 0.33                | 2.48       |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 20                  | 2.39     | 0.37                | 2.49       |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 20                  | 2.39     | 0.45                | 2.38       |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 20                  | 2.39     | 0.45                | 2.26       |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 20                  | 2.39     | 0.51                | 2.3        |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 20                  | 2.39     | 0.78                | 2.4        |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 20                  | 2.34     | 0.85                | 2.55       |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 20                  | 2.33     | 1.06                | 2.44       |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 20                  | 2.33     | 1.18                | 2.48       |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 20                  | 2.31     | 0.51                | 2.33       |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 20                  | 2.31     | 0.84                | 2.22       |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 20                  | 2.28     | 0.5                 | 2.33       |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 20                  | 2.28     | 0.84                | 2.12       |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 20                  | 2.27     | 0.26                | 2.26       |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 20                  | 2.25     | 0.45                | 2.34       |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 20                  | 2.24     | 0.83                | 2.36       |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 20                  | 2.2      | 0.68                | 1.96       |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 20                  | 2.18     | 1.08                | 2.2        |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 20                  | 2.16     | 0.43                | 2.09       |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 20                  | 2.16     | 0.47                | 2.16       |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 20                  | 2.16     | 0.19                | 2.16       |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 20                  | 2.11     | 0.3                 | 2.12       |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 20                  | 2.11     | 0.51                | 2.19       |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 20                  | 2.09     | 0.39                | 2.18       |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 20                  | 2.08     | 0.37                | 1.96       |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 20                  | 2.06     | 0.17                | 2.06       |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 20                  | 2.06     | 0.28                | 1.99       |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 20                  | 2.05     | 0.31                | 2.04       |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 20                  | 2.05     | 0.19                | 2.09       |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 20                  | 2.05     | 0.31                | 2.14       |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 20                  | 2.04     | 0.5                 | 2.0        |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 20                  | 2.01     | 0.26                | 2.01       |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 20                  | 2.0      | 0.17                | 2.06       |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 20                  | 1.99     | 0.63                | 1.84       |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 20                  | 1.97     | 0.69                | 1.8        |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 20                  | 1.93     | 0.48                | 1.84       |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 20                  | 1.92     | 0.74                | 1.9        |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 20                  | 1.88     | 0.65                | 1.86       |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 20                  | 1.86     | 0.29                | 1.87       |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 20                  | 1.86     | 0.28                | 2.0        |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 20                  | 1.84     | 0.48                | 1.74       |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 20                  | 1.84     | 0.81                | 1.7        |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 20                  | 1.83     | 0.51                | 1.8        |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 20                  | 1.81     | 0.9                 | 1.97       |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 20                  | 1.8      | 0.92                | 2.12       |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 20                  | 1.79     | 0.53                | 2.04       |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 20                  | 1.76     | 0.6                 | 1.84       |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 20                  | 1.74     | 1.01                | 1.47       |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 20                  | 1.72     | 0.16                | 1.74       |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 20                  | 1.72     | 0.19                | 1.76       |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 20                  | 1.69     | 0.51                | 1.78       |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 20                  | 1.67     | 0.57                | 1.67       |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 20                  | 1.66     | 0.3                 | 1.65       |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 20                  | 1.65     | 0.32                | 1.62       |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 20                  | 1.65     | 0.59                | 1.54       |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 20                  | 1.65     | 0.36                | 1.6        |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 20                  | 1.64     | 0.8                 | 1.61       |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 20                  | 1.63     | 0.57                | 1.73       |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 20                  | 1.61     | 0.29                | 1.6        |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 20                  | 1.58     | 1.08                | 1.33       |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 20                  | 1.56     | 0.99                | 1.44       |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 20                  | 1.52     | 0.32                | 1.56       |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 20                  | 1.49     | 0.45                | 1.48       |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 20                  | 1.47     | 0.09                | 1.45       |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 20                  | 1.47     | 0.41                | 1.46       |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 20                  | 1.46     | 0.65                | 1.25       |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 20                  | 1.44     | 0.27                | 1.38       |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 20                  | 1.43     | 0.6                 | 1.45       |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 20                  | 1.42     | 0.52                | 1.5        |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 20                  | 1.37     | 0.78                | 1.42       |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 20                  | 1.35     | 0.34                | 1.3        |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 20                  | 1.3      | 0.41                | 1.27       |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 20                  | 1.29     | 0.63                | 1.13       |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 20                  | 1.26     | 0.56                | 1.23       |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 20                  | 1.25     | 0.32                | 1.3        |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 20                  | 1.24     | 0.65                | 1.18       |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 20                  | 1.18     | 0.34                | 1.13       |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 20                  | 1.18     | 0.62                | 1.22       |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 20                  | 1.17     | 0.37                | 1.27       |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 20                  | 1.11     | 0.78                | 0.9        |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 20                  | 1.09     | 0.27                | 1.03       |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 20                  | 1.06     | 0.48                | 0.95       |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 20                  | 0.98     | 0.06                | 1.0        |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 20                  | 0.93     | 0.24                | 0.94       |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 20                  | 0.91     | 0.45                | 0.8        |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 20                  | 0.89     | 0.48                | 0.74       |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 20                  | 0.83     | 0.45                | 0.73       |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 20                  | 0.62     | 0.14                | 0.66       |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 20                  | 0.48     | 0.08                | 0.49       |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 20                  | 0.47     | 0.27                | 0.42       |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 20                  | 0.33     | 0.25                | 0.2        |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 20                  | 0.28     | 0.03                | 0.29       |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 20                  | 0.28     | 0.02                | 0.29       |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 20                  | 0.27     | 0.02                | 0.28       |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 20                  | 0.27     | 0.03                | 0.28       |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 20                  | 0.26     | 0.04                | 0.27       |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 20                  | 0.25     | 0.05                | 0.26       |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 20                  | 0.25     | 0.04                | 0.25       |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 20                  | 0.24     | 0.04                | 0.26       |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 20                  | 0.21     | 0.01                | 0.21       |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 20                  | 0.21     | 0.02                | 0.21       |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 20                  | 0.18     | 0.02                | 0.18       |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 19                  | 11.69    | 3.68                | 12.48      |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 19                  | 9.84     | 4.33                | 9.03       |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 19                  | 3.68     | 1.72                | 3.72       |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 19                  | 3.32     | 1.1                 | 3.23       |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 19                  | 2.97     | 1.64                | 2.35       |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 19                  | 2.94     | 0.65                | 3.03       |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 19                  | 2.49     | 0.93                | 2.28       |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 19                  | 1.72     | 1.31                | 1.27       |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 19                  | 1.04     | 0.74                | 0.93       |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 19                  | 1.0      | 0.35                | 1.01       |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 19                  | 0.87     | 0.6                 | 0.84       |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 19                  | 0.79     | 0.3                 | 0.78       |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 19                  | 0.56     | 0.25                | 0.49       |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 19                  | 0.23     | 0.05                | 0.25       |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 19                  | 0.23     | 0.04                | 0.23       |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 19                  | 0.16     | 0.04                | 0.15       |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 18                  | 3.42     | 2.68                | 2.36       |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 18                  | 2.83     | 1.05                | 2.93       |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 18                  | 2.47     | 1.37                | 2.28       |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 18                  | 2.31     | 1.27                | 2.46       |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 18                  | 2.25     | 1.75                | 1.72       |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 18                  | 2.23     | 1.17                | 2.1        |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 18                  | 1.88     | 0.92                | 2.17       |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 18                  | 1.48     | 0.73                | 1.5        |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 18                  | 1.1      | 0.72                | 0.84       |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 18                  | 0.82     | 0.29                | 0.8        |

*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) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 18                  | 0.74     | 0.3                 | 0.72       |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 18                  | 0.64     | 0.4                 | 0.52       |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 18                  | 0.26     | 0.05                | 0.28       |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 18                  | 0.24     | 0.05                | 0.25       |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 18                  | 0.22     | 0.05                | 0.24       |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 18                  | 0.22     | 0.03                | 0.21       |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 18                  | 0.22     | 0.05                | 0.24       |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 17                  | 3.32     | 1.28                | 3.4        |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 17                  | 1.54     | 0.92                | 1.18       |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 17                  | 1.39     | 0.73                | 1.61       |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 17                  | 0.51     | 0.3                 | 0.43       |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 17                  | 0.33     | 0.24                | 0.21       |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 17                  | 0.24     | 0.06                | 0.26       |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 17                  | 0.23     | 0.04                | 0.23       |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 17                  | 0.22     | 0.05                | 0.23       |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 17                  | 0.21     | 0.04                | 0.23       |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 17                  | 0.19     | 0.05                | 0.18       |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 17                  | 0.18     | 0.04                | 0.18       |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 16                  | 1.23     | 0.68                | 1.27       |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 16                  | 1.0      | 0.59                | 0.86       |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 16                  | 0.95     | 1.13                | 0.56       |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 16                  | 0.75     | 0.36                | 0.9        |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 16                  | 0.61     | 0.2                 | 0.66       |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 16                  | 0.38     | 0.22                | 0.41       |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 16                  | 0.26     | 0.04                | 0.27       |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 16                  | 0.21     | 0.04                | 0.22       |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 16                  | 0.21     | 0.06                | 0.2        |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 15                  | 0.86     | 0.52                | 0.94       |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 15                  | 0.3      | 0.09                | 0.28       |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 15                  | 0.27     | 0.06                | 0.3        |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 14                  | 0.28     | 0.04                | 0.3        |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 14                  | 0.22     | 0.12                | 0.19       |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 14                  | 0.2      | 0.06                | 0.2        |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 13                  | 1.67     | 0.72                | 1.8        |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 13                  | 0.63     | 0.32                | 0.56       |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 13                  | 0.5      | 0.4                 | 0.36       |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 13                  | 0.44     | 0.25                | 0.34       |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 13                  | 0.27     | 0.21                | 0.22       |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 12                  | 0.89     | 0.49                | 0.84       |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 12                  | 0.47     | 0.38                | 0.4        |
| (1,514) | 1:20:A:TYR:CB | 1:92:A:LEU:H  | 10                  | 0.76     | 0.48                | 0.68       |
| (3,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 10                  | 0.2      | 0.05                | 0.2        |

*Continued on next page...*

*Continued from previous page...*

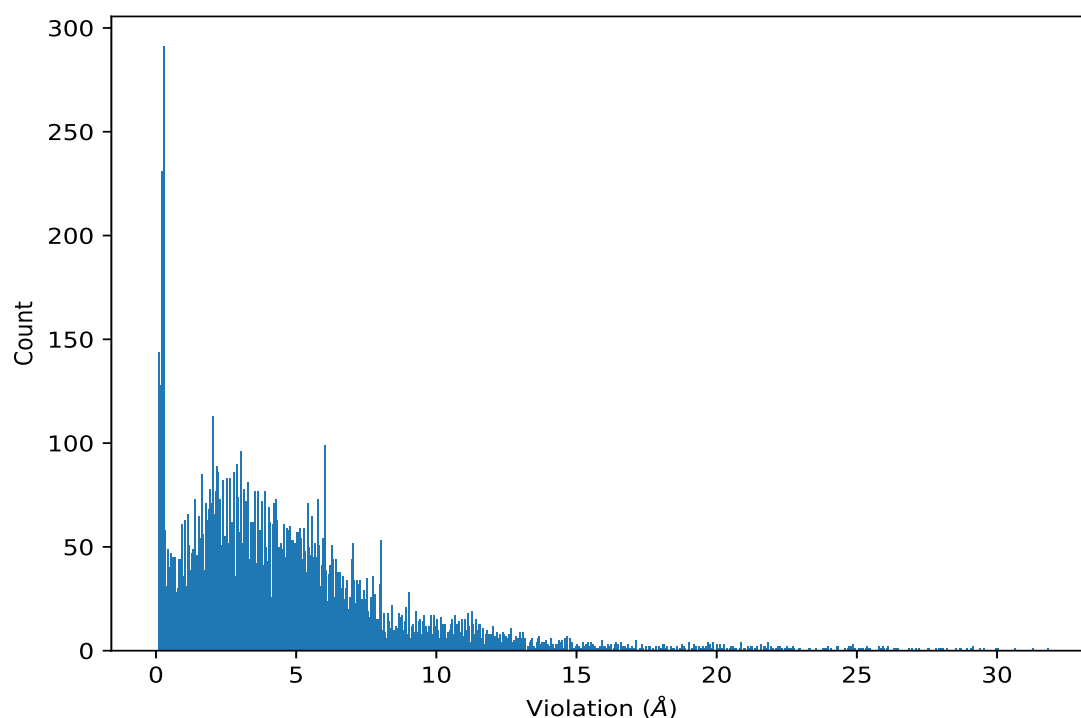
| Key     | Atom-1        | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|---------------|---------------------|----------|---------------------|------------|
| (4,16)  | 1:33:A:LEU:O  | 1:37:A:CYS:N  | 10                  | 0.18     | 0.04                | 0.2        |
| (1,567) | 1:30:A:ILE:H  | 1:56:A:SER:CB | 9                   | 0.37     | 0.17                | 0.38       |
| (4,34)  | 1:90:A:MET:O  | 1:94:A:LEU:N  | 8                   | 0.12     | 0.02                | 0.12       |
| (4,11)  | 1:38:A:LEU:O  | 1:42:A:GLY:N  | 7                   | 0.2      | 0.07                | 0.2        |
| (4,10)  | 1:39:A:ALA:O  | 1:43:A:ALA:N  | 6                   | 0.22     | 0.06                | 0.22       |
| (4,3)   | 1:13:A:THR:O  | 1:17:A:ILE:N  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,645) | 1:41:A:TYR:H  | 1:56:A:SER:CB | 5                   | 0.25     | 0.09                | 0.23       |
| (4,4)   | 1:12:A:VAL:O  | 1:16:A:SER:N  | 5                   | 0.18     | 0.05                | 0.2        |
| (4,23)  | 1:63:A:LEU:O  | 1:67:A:MET:N  | 5                   | 0.15     | 0.02                | 0.13       |
| (4,20)  | 1:29:A:LEU:O  | 1:33:A:LEU:N  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,226) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 4                   | 0.23     | 0.1                 | 0.22       |
| (4,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:N  | 4                   | 0.22     | 0.09                | 0.21       |
| (4,24)  | 1:62:A:PHE:O  | 1:66:A:ILE:N  | 4                   | 0.19     | 0.03                | 0.18       |
| (1,797) | 1:74:A:SER:CB | 1:90:A:MET:H  | 4                   | 0.15     | 0.03                | 0.15       |
| (1,609) | 1:37:A:CYS:CB | 1:63:A:LEU:H  | 2                   | 0.28     | 0.08                | 0.28       |
| (4,87)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 2                   | 0.15     | 0.03                | 0.15       |
| (4,43)  | 1:81:A:GLY:O  | 1:85:A:GLY:N  | 2                   | 0.11     | 0.0                 | 0.11       |

<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) |
|---------|-------------|---------------|----------|---------------|
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 9        | 31.83         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 9        | 31.26         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 6        | 30.62         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 20       | 30.02         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 19       | 29.99         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 20       | 29.52         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 8        | 29.36         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 9        | 29.1          |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 19       | 29.1          |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 6        | 29.06         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 13       | 28.94         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 7        | 28.73         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 8        | 28.68         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 18       | 28.53         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 7        | 28.21         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 10       | 28.07         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1      | Atom-2        | Model ID | Violation (Å) |
|---------|-------------|---------------|----------|---------------|
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 20       | 28.01         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 18       | 27.98         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 2        | 27.95         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 10       | 27.82         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 2        | 27.56         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 1        | 27.53         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 8        | 27.21         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 1        | 27.14         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 17       | 26.99         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 7        | 26.9          |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 15       | 26.48         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 6        | 26.43         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 17       | 26.38         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 2        | 26.33         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 11       | 26.15         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 19       | 26.14         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 20       | 26.09         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 18       | 25.98         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 13       | 25.95         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 1        | 25.92         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 7        | 25.87         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 8        | 25.8          |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 2        | 25.76         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 15       | 25.75         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 9        | 25.49         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 17       | 25.44         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 3        | 25.36         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 12       | 25.35         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 18       | 25.31         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 14       | 25.21         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 15       | 25.19         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 3        | 25.13         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 10       | 25.08         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 1        | 24.94         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 11       | 24.9          |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 12       | 24.87         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 3        | 24.85         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 12       | 24.79         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 13       | 24.76         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 6        | 24.71         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 15       | 24.71         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 10       | 24.69         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1      | Atom-2        | Model ID | Violation (Å) |
|---------|-------------|---------------|----------|---------------|
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 5        | 24.55         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 19       | 24.32         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 3        | 24.31         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 17       | 24.29         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 8        | 24.25         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 16       | 24.08         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 4        | 23.98         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 12       | 23.96         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 9        | 23.94         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 7        | 23.88         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 20       | 23.83         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 14       | 23.78         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 11       | 23.52         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 2        | 23.34         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 18       | 23.28         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 11       | 22.98         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 1        | 22.92         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 13       | 22.78         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 14       | 22.72         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 10       | 22.71         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 4        | 22.7          |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 4        | 22.64         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 15       | 22.57         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 17       | 22.53         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 14       | 22.5          |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 8        | 22.41         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 14       | 22.32         |
| (1,359) | 1:5:A:GLY:H | 1:47:A:SER:CB | 5        | 22.28         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 14       | 22.27         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 9        | 22.2          |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 8        | 22.19         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 7        | 22.14         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 9        | 22.03         |
| (1,339) | 1:2:A:ASP:H | 1:47:A:SER:CB | 4        | 21.95         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 20       | 21.92         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 6        | 21.83         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 5        | 21.83         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 19       | 21.82         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 3        | 21.8          |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 12       | 21.77         |
| (1,346) | 1:3:A:LEU:H | 1:56:A:SER:CB | 9        | 21.74         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 18       | 21.71         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1      | Atom-2        | Model ID | Violation (Å) |
|---------|-------------|---------------|----------|---------------|
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 7        | 21.68         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 18       | 21.66         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 14       | 21.59         |
| (1,360) | 1:5:A:GLY:H | 1:56:A:SER:CB | 2        | 21.59         |
| (1,352) | 1:4:A:ILE:H | 1:47:A:SER:CB | 16       | 21.56         |
| (1,360) | 1:5:A:GLY:H | 1:56:A:SER:CB | 20       | 21.42         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 5        | 21.41         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 20       | 21.37         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 10       | 21.27         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 5        | 21.27         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 15       | 21.21         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 2        | 21.21         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 1        | 21.17         |
| (1,360) | 1:5:A:GLY:H | 1:56:A:SER:CB | 7        | 21.15         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 1        | 21.12         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 10       | 21.03         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 15       | 20.96         |
| (1,387) | 1:9:A:ALA:H | 1:47:A:SER:CB | 8        | 20.9          |
| (1,340) | 1:2:A:ASP:H | 1:56:A:SER:CB | 6        | 20.88         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 2        | 20.87         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 13       | 20.86         |
| (1,346) | 1:3:A:LEU:H | 1:56:A:SER:CB | 6        | 20.84         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 17       | 20.66         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 5        | 20.65         |
| (1,360) | 1:5:A:GLY:H | 1:56:A:SER:CB | 8        | 20.58         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 5        | 20.57         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 4        | 20.52         |
| (1,387) | 1:9:A:ALA:H | 1:47:A:SER:CB | 9        | 20.5          |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 17       | 20.47         |
| (1,346) | 1:3:A:LEU:H | 1:56:A:SER:CB | 20       | 20.35         |
| (1,366) | 1:6:A:PHE:H | 1:47:A:SER:CB | 11       | 20.29         |
| (1,387) | 1:9:A:ALA:H | 1:47:A:SER:CB | 7        | 20.27         |
| (1,345) | 1:3:A:LEU:H | 1:47:A:SER:CB | 16       | 20.25         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 3        | 20.19         |
| (1,387) | 1:9:A:ALA:H | 1:47:A:SER:CB | 18       | 20.14         |
| (1,387) | 1:9:A:ALA:H | 1:47:A:SER:CB | 20       | 20.13         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 3        | 20.1          |
| (1,360) | 1:5:A:GLY:H | 1:56:A:SER:CB | 10       | 20.07         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 12       | 20.04         |
| (1,368) | 1:6:A:PHE:H | 1:74:A:SER:CB | 16       | 20.04         |
| (1,380) | 1:8:A:TYR:H | 1:47:A:SER:CB | 19       | 20.03         |
| (1,373) | 1:7:A:GLY:H | 1:47:A:SER:CB | 19       | 19.9          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,373) | 1:7:A:GLY:H  | 1:47:A:SER:CB | 16       | 19.88         |
| (1,340) | 1:2:A:ASP:H  | 1:56:A:SER:CB | 9        | 19.87         |
| (1,346) | 1:3:A:LEU:H  | 1:56:A:SER:CB | 10       | 19.86         |
| (1,375) | 1:7:A:GLY:H  | 1:74:A:SER:CB | 16       | 19.8          |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 6        | 19.77         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 2        | 19.76         |
| (1,346) | 1:3:A:LEU:H  | 1:56:A:SER:CB | 19       | 19.75         |
| (1,366) | 1:6:A:PHE:H  | 1:47:A:SER:CB | 16       | 19.72         |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 1        | 19.71         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 15       | 19.69         |
| (1,380) | 1:8:A:TYR:H  | 1:47:A:SER:CB | 13       | 19.67         |
| (1,373) | 1:7:A:GLY:H  | 1:47:A:SER:CB | 12       | 19.67         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 1        | 19.66         |
| (1,380) | 1:8:A:TYR:H  | 1:47:A:SER:CB | 6        | 19.6          |
| (1,373) | 1:7:A:GLY:H  | 1:47:A:SER:CB | 6        | 19.6          |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 17       | 19.58         |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 9        | 19.53         |
| (1,340) | 1:2:A:ASP:H  | 1:56:A:SER:CB | 20       | 19.52         |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 17       | 19.44         |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 12       | 19.39         |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 3        | 19.35         |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 15       | 19.29         |
| (1,373) | 1:7:A:GLY:H  | 1:47:A:SER:CB | 13       | 19.27         |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 11       | 19.19         |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 19       | 19.19         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 10       | 19.17         |
| (1,380) | 1:8:A:TYR:H  | 1:47:A:SER:CB | 4        | 19.13         |
| (1,380) | 1:8:A:TYR:H  | 1:47:A:SER:CB | 16       | 19.04         |
| (1,340) | 1:2:A:ASP:H  | 1:56:A:SER:CB | 19       | 19.04         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 12       | 19.03         |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 18       | 19.02         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 19       | 18.88         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 14       | 18.84         |
| (1,346) | 1:3:A:LEU:H  | 1:56:A:SER:CB | 8        | 18.8          |
| (1,373) | 1:7:A:GLY:H  | 1:47:A:SER:CB | 4        | 18.76         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 3        | 18.75         |
| (1,353) | 1:4:A:ILE:H  | 1:56:A:SER:CB | 20       | 18.75         |
| (1,341) | 1:2:A:ASP:H  | 1:74:A:SER:CB | 6        | 18.69         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 8        | 18.59         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 6        | 18.58         |
| (1,380) | 1:8:A:TYR:H  | 1:47:A:SER:CB | 11       | 18.48         |
| (1,354) | 1:4:A:ILE:H  | 1:74:A:SER:CB | 16       | 18.41         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,359) | 1:5:A:GLY:H  | 1:47:A:SER:CB | 16       | 18.37         |
| (1,346) | 1:3:A:LEU:H  | 1:56:A:SER:CB | 7        | 18.36         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 5        | 18.22         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 9        | 18.21         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 13       | 18.16         |
| (1,373) | 1:7:A:GLY:H  | 1:47:A:SER:CB | 11       | 18.14         |
| (1,353) | 1:4:A:ILE:H  | 1:56:A:SER:CB | 9        | 18.12         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 14       | 18.1          |
| (1,349) | 1:3:A:LEU:H  | 1:99:A:LEU:CB | 9        | 18.09         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 7        | 18.07         |
| (1,347) | 1:3:A:LEU:H  | 1:74:A:SER:CB | 6        | 18.07         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 14       | 18.02         |
| (1,340) | 1:2:A:ASP:H  | 1:56:A:SER:CB | 10       | 17.97         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 20       | 17.93         |
| (1,346) | 1:3:A:LEU:H  | 1:56:A:SER:CB | 2        | 17.91         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 18       | 17.82         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 4        | 17.82         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 8        | 17.73         |
| (1,349) | 1:3:A:LEU:H  | 1:99:A:LEU:CB | 10       | 17.64         |
| (1,346) | 1:3:A:LEU:H  | 1:56:A:SER:CB | 18       | 17.64         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 9        | 17.59         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 11       | 17.55         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 9        | 17.49         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 2        | 17.45         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 1        | 17.39         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 8        | 17.33         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 18       | 17.32         |
| (1,361) | 1:5:A:GLY:H  | 1:74:A:SER:CB | 16       | 17.31         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 15       | 17.29         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 7        | 17.14         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 10       | 17.14         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 18       | 17.12         |
| (1,353) | 1:4:A:ILE:H  | 1:56:A:SER:CB | 7        | 17.12         |
| (1,353) | 1:4:A:ILE:H  | 1:56:A:SER:CB | 8        | 17.11         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 17       | 17.08         |
| (1,361) | 1:5:A:GLY:H  | 1:74:A:SER:CB | 2        | 17.04         |
| (1,349) | 1:3:A:LEU:H  | 1:99:A:LEU:CB | 18       | 16.98         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 15       | 16.97         |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 4        | 16.92         |
| (1,382) | 1:8:A:TYR:H  | 1:74:A:SER:CB | 16       | 16.89         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 20       | 16.83         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 5        | 16.82         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,353) | 1:4:A:ILE:H  | 1:56:A:SER:CB | 6        | 16.81         |
| (1,340) | 1:2:A:ASP:H  | 1:56:A:SER:CB | 8        | 16.78         |
| (1,349) | 1:3:A:LEU:H  | 1:99:A:LEU:CB | 20       | 16.74         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 1        | 16.72         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 15       | 16.69         |
| (1,340) | 1:2:A:ASP:H  | 1:56:A:SER:CB | 7        | 16.66         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 10       | 16.62         |
| (1,349) | 1:3:A:LEU:H  | 1:99:A:LEU:CB | 19       | 16.62         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 5        | 16.58         |
| (1,361) | 1:5:A:GLY:H  | 1:74:A:SER:CB | 11       | 16.57         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 7        | 16.56         |
| (1,347) | 1:3:A:LEU:H  | 1:74:A:SER:CB | 19       | 16.55         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 14       | 16.49         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 1        | 16.48         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 12       | 16.47         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 17       | 16.43         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 19       | 16.42         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 2        | 16.41         |
| (1,353) | 1:4:A:ILE:H  | 1:56:A:SER:CB | 2        | 16.41         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 17       | 16.4          |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 3        | 16.39         |
| (1,347) | 1:3:A:LEU:H  | 1:74:A:SER:CB | 9        | 16.37         |
| (1,396) | 1:10:A:ALA:H | 1:74:A:SER:CB | 16       | 16.33         |
| (1,344) | 1:3:A:LEU:H  | 1:37:A:CYS:CB | 9        | 16.23         |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 13       | 16.22         |
| (1,342) | 1:2:A:ASP:H  | 1:87:A:SER:CB | 6        | 16.21         |
| (1,387) | 1:9:A:ALA:H  | 1:47:A:SER:CB | 16       | 16.18         |
| (1,341) | 1:2:A:ASP:H  | 1:74:A:SER:CB | 19       | 16.17         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 10       | 16.12         |
| (1,394) | 1:10:A:ALA:H | 1:47:A:SER:CB | 6        | 16.12         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 20       | 16.11         |
| (1,340) | 1:2:A:ASP:H  | 1:56:A:SER:CB | 2        | 16.08         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 5        | 16.02         |
| (1,346) | 1:3:A:LEU:H  | 1:56:A:SER:CB | 1        | 16.0          |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 16       | 15.99         |
| (1,382) | 1:8:A:TYR:H  | 1:74:A:SER:CB | 7        | 15.98         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 2        | 15.93         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 12       | 15.93         |
| (1,349) | 1:3:A:LEU:H  | 1:99:A:LEU:CB | 6        | 15.93         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 12       | 15.91         |
| (1,348) | 1:3:A:LEU:H  | 1:87:A:SER:CB | 9        | 15.9          |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 3        | 15.88         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 11       | 15.87         |
| (1,346) | 1:3:A:LEU:H   | 1:56:A:SER:CB | 11       | 15.83         |
| (1,394) | 1:10:A:ALA:H  | 1:47:A:SER:CB | 16       | 15.81         |
| (1,394) | 1:10:A:ALA:H  | 1:47:A:SER:CB | 13       | 15.78         |
| (1,401) | 1:11:A:LEU:H  | 1:47:A:SER:CB | 19       | 15.73         |
| (1,407) | 1:12:A:VAL:H  | 1:47:A:SER:CB | 19       | 15.67         |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 19       | 15.67         |
| (1,407) | 1:12:A:VAL:H  | 1:47:A:SER:CB | 3        | 15.62         |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 20       | 15.58         |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 10       | 15.58         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 16       | 15.57         |
| (1,401) | 1:11:A:LEU:H  | 1:47:A:SER:CB | 13       | 15.54         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 2        | 15.54         |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 16       | 15.54         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 4        | 15.52         |
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 8        | 15.46         |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 10       | 15.46         |
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 2        | 15.45         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 6        | 15.44         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 8        | 15.43         |
| (1,407) | 1:12:A:VAL:H  | 1:47:A:SER:CB | 13       | 15.4          |
| (1,394) | 1:10:A:ALA:H  | 1:47:A:SER:CB | 4        | 15.36         |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 9        | 15.36         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 9        | 15.35         |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 19       | 15.32         |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 9        | 15.3          |
| (1,401) | 1:11:A:LEU:H  | 1:47:A:SER:CB | 6        | 15.28         |
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 18       | 15.25         |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 7        | 15.24         |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 6        | 15.23         |
| (1,407) | 1:12:A:VAL:H  | 1:47:A:SER:CB | 6        | 15.22         |
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 13       | 15.22         |
| (1,360) | 1:5:A:GLY:H   | 1:56:A:SER:CB | 14       | 15.19         |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 16       | 15.08         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 17       | 15.05         |
| (1,401) | 1:11:A:LEU:H  | 1:47:A:SER:CB | 4        | 15.01         |
| (1,394) | 1:10:A:ALA:H  | 1:47:A:SER:CB | 11       | 15.01         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 18       | 15.0          |
| (1,407) | 1:12:A:VAL:H  | 1:47:A:SER:CB | 4        | 14.99         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 19       | 14.96         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 20       | 14.95         |
| (1,346) | 1:3:A:LEU:H   | 1:56:A:SER:CB | 17       | 14.86         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (1,363) | 1:5:A:GLY:H  | 1:99:A:LEU:CB | 2        | 14.85         |
| (1,349) | 1:3:A:LEU:H  | 1:99:A:LEU:CB | 1        | 14.83         |
| (1,349) | 1:3:A:LEU:H  | 1:99:A:LEU:CB | 3        | 14.83         |
| (1,403) | 1:11:A:LEU:H | 1:74:A:SER:CB | 16       | 14.8          |
| (1,704) | 1:48:A:ASN:H | 1:74:A:SER:CB | 8        | 14.79         |
| (1,354) | 1:4:A:ILE:H  | 1:74:A:SER:CB | 7        | 14.79         |
| (1,413) | 1:13:A:THR:H | 1:47:A:SER:CB | 20       | 14.78         |
| (1,363) | 1:5:A:GLY:H  | 1:99:A:LEU:CB | 20       | 14.78         |
| (1,368) | 1:6:A:PHE:H  | 1:74:A:SER:CB | 7        | 14.77         |
| (1,413) | 1:13:A:THR:H | 1:47:A:SER:CB | 18       | 14.76         |
| (1,375) | 1:7:A:GLY:H  | 1:74:A:SER:CB | 7        | 14.7          |
| (1,342) | 1:2:A:ASP:H  | 1:87:A:SER:CB | 10       | 14.7          |
| (1,360) | 1:5:A:GLY:H  | 1:56:A:SER:CB | 5        | 14.69         |
| (1,413) | 1:13:A:THR:H | 1:47:A:SER:CB | 7        | 14.68         |
| (1,349) | 1:3:A:LEU:H  | 1:99:A:LEU:CB | 7        | 14.67         |
| (1,346) | 1:3:A:LEU:H  | 1:56:A:SER:CB | 3        | 14.66         |
| (1,375) | 1:7:A:GLY:H  | 1:74:A:SER:CB | 11       | 14.65         |
| (1,363) | 1:5:A:GLY:H  | 1:99:A:LEU:CB | 3        | 14.64         |
| (1,375) | 1:7:A:GLY:H  | 1:74:A:SER:CB | 2        | 14.6          |
| (1,413) | 1:13:A:THR:H | 1:47:A:SER:CB | 2        | 14.58         |
| (1,367) | 1:6:A:PHE:H  | 1:56:A:SER:CB | 7        | 14.58         |
| (1,368) | 1:6:A:PHE:H  | 1:74:A:SER:CB | 2        | 14.57         |
| (1,354) | 1:4:A:ILE:H  | 1:74:A:SER:CB | 6        | 14.57         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 11       | 14.56         |
| (1,368) | 1:6:A:PHE:H  | 1:74:A:SER:CB | 11       | 14.51         |
| (1,346) | 1:3:A:LEU:H  | 1:56:A:SER:CB | 13       | 14.49         |
| (1,413) | 1:13:A:THR:H | 1:47:A:SER:CB | 15       | 14.48         |
| (1,356) | 1:4:A:ILE:H  | 1:99:A:LEU:CB | 9        | 14.48         |
| (1,704) | 1:48:A:ASN:H | 1:74:A:SER:CB | 17       | 14.47         |
| (1,407) | 1:12:A:VAL:H | 1:47:A:SER:CB | 16       | 14.46         |
| (1,346) | 1:3:A:LEU:H  | 1:56:A:SER:CB | 15       | 14.45         |
| (1,413) | 1:13:A:THR:H | 1:47:A:SER:CB | 17       | 14.44         |
| (1,363) | 1:5:A:GLY:H  | 1:99:A:LEU:CB | 7        | 14.41         |
| (1,413) | 1:13:A:THR:H | 1:47:A:SER:CB | 1        | 14.4          |
| (1,681) | 1:47:A:SER:H | 1:74:A:SER:CB | 15       | 14.39         |
| (1,363) | 1:5:A:GLY:H  | 1:99:A:LEU:CB | 10       | 14.37         |
| (1,354) | 1:4:A:ILE:H  | 1:74:A:SER:CB | 2        | 14.37         |
| (1,401) | 1:11:A:LEU:H | 1:47:A:SER:CB | 11       | 14.36         |
| (1,347) | 1:3:A:LEU:H  | 1:74:A:SER:CB | 20       | 14.36         |
| (1,424) | 1:15:A:GLY:H | 1:47:A:SER:CB | 14       | 14.32         |
| (1,342) | 1:2:A:ASP:H  | 1:87:A:SER:CB | 19       | 14.31         |
| (1,342) | 1:2:A:ASP:H  | 1:87:A:SER:CB | 20       | 14.3          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 15       | 14.27         |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 9        | 14.27         |
| (1,360) | 1:5:A:GLY:H   | 1:56:A:SER:CB | 16       | 14.26         |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 20       | 14.23         |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 15       | 14.18         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 19       | 14.17         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 13       | 14.15         |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 19       | 14.14         |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 18       | 14.13         |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 20       | 14.13         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 8        | 14.1          |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 20       | 14.09         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 20       | 14.07         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 14       | 14.06         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 14       | 14.06         |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 20       | 14.06         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 2        | 14.01         |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 19       | 14.01         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 11       | 13.96         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 1        | 13.96         |
| (1,346) | 1:3:A:LEU:H   | 1:56:A:SER:CB | 12       | 13.96         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 15       | 13.94         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 12       | 13.94         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 7        | 13.94         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 10       | 13.92         |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 17       | 13.91         |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 6        | 13.86         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 8        | 13.82         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 7        | 13.82         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 14       | 13.8          |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 12       | 13.8          |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 19       | 13.77         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 17       | 13.77         |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 14       | 13.75         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 10       | 13.75         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 14       | 13.74         |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 8        | 13.74         |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 10       | 13.73         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 9        | 13.7          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 16       | 13.69         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 11       | 13.69         |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 7        | 13.69         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 8        | 13.68         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 20       | 13.68         |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 13       | 13.67         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 8        | 13.62         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 11       | 13.62         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 7        | 13.62         |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 12       | 13.62         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 8        | 13.62         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 7        | 13.61         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 3        | 13.59         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 7        | 13.59         |
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 1        | 13.59         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 9        | 13.55         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 20       | 13.52         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 2        | 13.49         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 3        | 13.46         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 8        | 13.45         |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 8        | 13.45         |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 2        | 13.45         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 17       | 13.44         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 11       | 13.44         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 9        | 13.4          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 11       | 13.39         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 16       | 13.39         |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 8        | 13.39         |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 1        | 13.37         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 6        | 13.36         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 18       | 13.34         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 5        | 13.31         |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 2        | 13.3          |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 3        | 13.3          |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 4        | 13.29         |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 1        | 13.28         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 12       | 13.2          |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 12       | 13.2          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 9        | 13.17         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 6        | 13.16         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 18       | 13.16         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 10       | 13.15         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 13       | 13.14         |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 7        | 13.13         |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 11       | 13.1          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 6        | 13.09         |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 17       | 13.08         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 9        | 13.08         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 11       | 13.07         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 20       | 13.07         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 5        | 13.06         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 15       | 13.06         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 10       | 13.05         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 2        | 13.04         |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 4        | 13.03         |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 11       | 13.03         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 19       | 13.02         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 8        | 13.0          |
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 17       | 13.0          |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 8        | 12.99         |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 17       | 12.99         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 4        | 12.98         |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 7        | 12.98         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 9        | 12.97         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 11       | 12.97         |
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 3        | 12.97         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 9        | 12.96         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 17       | 12.96         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 6        | 12.94         |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 13       | 12.94         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 2        | 12.93         |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 18       | 12.93         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 4        | 12.91         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 5        | 12.9          |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 8        | 12.89         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 1        | 12.88         |
| (1,346) | 1:3:A:LEU:H   | 1:56:A:SER:CB | 4        | 12.88         |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 4        | 12.87         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 19       | 12.87         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 12       | 12.87         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 8        | 12.85         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 8        | 12.85         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 19       | 12.85         |
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 17       | 12.85         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 6        | 12.84         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 2        | 12.83         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 10       | 12.8          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 18       | 12.79         |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 11       | 12.79         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 18       | 12.76         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 6        | 12.75         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 9        | 12.75         |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 20       | 12.74         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 4        | 12.72         |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 9        | 12.71         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 7        | 12.71         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 13       | 12.69         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 7        | 12.68         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 16       | 12.68         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 3        | 12.67         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 15       | 12.67         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 9        | 12.67         |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 19       | 12.67         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 10       | 12.66         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 17       | 12.66         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 15       | 12.65         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 9        | 12.65         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 20       | 12.64         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 11       | 12.63         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 14       | 12.62         |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 15       | 12.62         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 8        | 12.6          |
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 13       | 12.6          |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 16       | 12.59         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 20       | 12.58         |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 6        | 12.57         |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 15       | 12.56         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 2        | 12.56         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 19       | 12.56         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 15       | 12.53         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 10       | 12.52         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 20       | 12.51         |
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 11       | 12.51         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 1        | 12.51         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 16       | 12.5          |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 7        | 12.48         |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 10       | 12.48         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 5        | 12.47         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 20       | 12.47         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 3        | 12.47         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 14       | 12.46         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 15       | 12.46         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 15       | 12.45         |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 19       | 12.44         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 12       | 12.44         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 17       | 12.43         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 1        | 12.42         |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 2        | 12.42         |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 3        | 12.41         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 15       | 12.4          |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 18       | 12.39         |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 11       | 12.39         |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 17       | 12.39         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 7        | 12.39         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 14       | 12.39         |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 16       | 12.38         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 10       | 12.36         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 17       | 12.36         |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 2        | 12.36         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 18       | 12.35         |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 20       | 12.33         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 18       | 12.3          |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 5        | 12.3          |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 8        | 12.29         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 4        | 12.28         |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 17       | 12.28         |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 11       | 12.28         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 7        | 12.27         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 1        | 12.27         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 15       | 12.26         |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 7        | 12.26         |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 11       | 12.24         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 17       | 12.23         |
| (1,413) | 1:13:A:THR:H  | 1:47:A:SER:CB | 16       | 12.22         |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 8        | 12.22         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 11       | 12.21         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 15       | 12.21         |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 2        | 12.2          |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 2        | 12.2          |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 8        | 12.19         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 1        | 12.17         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 16       | 12.17         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 10       | 12.16         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 19       | 12.16         |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 7        | 12.16         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 11       | 12.15         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 2        | 12.14         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 6        | 12.12         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 7        | 12.12         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 17       | 12.1          |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 8        | 12.09         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 16       | 12.08         |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 20       | 12.08         |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 19       | 12.06         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 19       | 12.06         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 19       | 12.05         |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 5        | 12.04         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 17       | 12.04         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 3        | 12.04         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 19       | 12.03         |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 12       | 12.03         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 20       | 12.03         |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 12       | 12.02         |
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 11       | 12.02         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 13       | 12.01         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 6        | 12.01         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 13       | 12.01         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 17       | 12.0          |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 17       | 11.99         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 12       | 11.99         |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 2        | 11.98         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 12       | 11.98         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 5        | 11.97         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 1        | 11.97         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 9        | 11.97         |
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 15       | 11.96         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 7        | 11.95         |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 4        | 11.95         |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 19       | 11.95         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 12       | 11.94         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 1        | 11.94         |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 7        | 11.94         |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 9        | 11.94         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 17       | 11.93         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 1        | 11.89         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 10       | 11.89         |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 2        | 11.87         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 9        | 11.87         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 17       | 11.87         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 1        | 11.86         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 19       | 11.86         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 8        | 11.86         |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 4        | 11.85         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 14       | 11.84         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 7        | 11.84         |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 16       | 11.84         |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 15       | 11.83         |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 4        | 11.83         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 17       | 11.83         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 17       | 11.83         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 8        | 11.82         |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 13       | 11.81         |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 15       | 11.79         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 5        | 11.79         |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 2        | 11.79         |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 11       | 11.78         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 15       | 11.77         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 4        | 11.77         |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 3        | 11.76         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 19       | 11.75         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 12       | 11.72         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 2        | 11.71         |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 9        | 11.71         |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 7        | 11.7          |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 15       | 11.7          |
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 12       | 11.7          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 20       | 11.7          |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 9        | 11.69         |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 15       | 11.69         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 20       | 11.69         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 9        | 11.68         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 10       | 11.68         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 20       | 11.68         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 4        | 11.66         |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 17       | 11.64         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 20       | 11.64         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 16       | 11.63         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 1        | 11.62         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 1        | 11.62         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 11       | 11.62         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 18       | 11.6          |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 4        | 11.6          |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 15       | 11.6          |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 5        | 11.59         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 13       | 11.59         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 13       | 11.57         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 13       | 11.56         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 12       | 11.56         |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 18       | 11.56         |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 2        | 11.56         |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 13       | 11.55         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 16       | 11.55         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 12       | 11.55         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 19       | 11.54         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 6        | 11.53         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 15       | 11.53         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 6        | 11.53         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 1        | 11.53         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 6        | 11.52         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 17       | 11.52         |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 20       | 11.52         |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 8        | 11.51         |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 2        | 11.51         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 5        | 11.51         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 13       | 11.5          |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 7        | 11.5          |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 11       | 11.49         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 15       | 11.49         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 4        | 11.49         |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 10       | 11.49         |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 1        | 11.49         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 3        | 11.48         |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 8        | 11.47         |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 2        | 11.47         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 4        | 11.46         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 12       | 11.46         |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 11       | 11.45         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 19       | 11.45         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 20       | 11.45         |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 8        | 11.44         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 6        | 11.44         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 12       | 11.43         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 17       | 11.42         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 2        | 11.42         |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 10       | 11.41         |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 10       | 11.41         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 6        | 11.41         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 13       | 11.41         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 18       | 11.41         |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 15       | 11.4          |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 13       | 11.4          |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 13       | 11.39         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 6        | 11.39         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 17       | 11.38         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 15       | 11.38         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 2        | 11.37         |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 8        | 11.37         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 15       | 11.36         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 19       | 11.36         |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 7        | 11.35         |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 18       | 11.35         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 8        | 11.35         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 15       | 11.35         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 19       | 11.35         |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 7        | 11.35         |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 9        | 11.34         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 19       | 11.33         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 10       | 11.32         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 3        | 11.3          |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 3        | 11.3          |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 9        | 11.3          |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 3        | 11.3          |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 3        | 11.29         |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 4        | 11.29         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 19       | 11.29         |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 6        | 11.28         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 1        | 11.28         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 13       | 11.28         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 8        | 11.28         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 10       | 11.28         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 17       | 11.28         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 3        | 11.27         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 1        | 11.27         |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 8        | 11.27         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 15       | 11.27         |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 2        | 11.26         |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 12       | 11.26         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 13       | 11.26         |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 2        | 11.25         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 1        | 11.25         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 9        | 11.25         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 16       | 11.24         |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 17       | 11.22         |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 2        | 11.21         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 6        | 11.21         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 6        | 11.2          |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 6        | 11.2          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 20       | 11.19         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 2        | 11.19         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 11       | 11.17         |
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 4        | 11.17         |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 7        | 11.17         |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 9        | 11.16         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 9        | 11.15         |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 13       | 11.15         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 3        | 11.15         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 13       | 11.15         |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 4        | 11.14         |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 1        | 11.14         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 13       | 11.14         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 1        | 11.14         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 20       | 11.14         |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 17       | 11.13         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 11       | 11.13         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 4        | 11.13         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 6        | 11.12         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 4        | 11.12         |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 7        | 11.12         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 12       | 11.12         |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 11       | 11.11         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 16       | 11.11         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 7        | 11.11         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 6        | 11.11         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 1        | 11.11         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 13       | 11.11         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 7        | 11.1          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 8        | 11.1          |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 17       | 11.1          |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 1        | 11.08         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 12       | 11.08         |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 20       | 11.08         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 6        | 11.08         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 1        | 11.08         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 6        | 11.06         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 14       | 11.06         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 4        | 11.04         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 6        | 11.04         |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 20       | 11.03         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 13       | 11.03         |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 4        | 11.03         |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 8        | 11.03         |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 8        | 11.03         |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 3        | 11.02         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 3        | 11.02         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 12       | 11.02         |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 14       | 11.01         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 5        | 11.01         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 18       | 11.01         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 2        | 11.0          |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 2        | 11.0          |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 10       | 10.99         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 14       | 10.98         |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 4        | 10.98         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 2        | 10.97         |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 2        | 10.97         |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 7        | 10.97         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 20       | 10.96         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 14       | 10.95         |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 12       | 10.95         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 3        | 10.94         |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 11       | 10.94         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 6        | 10.93         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 13       | 10.93         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 3        | 10.92         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 3        | 10.92         |
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 16       | 10.92         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 12       | 10.91         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 4        | 10.91         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 8        | 10.91         |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 16       | 10.9          |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 4        | 10.9          |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 10       | 10.9          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 9        | 10.89         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 11       | 10.88         |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 3        | 10.88         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 2        | 10.88         |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 15       | 10.88         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 19       | 10.88         |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 11       | 10.87         |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 3        | 10.87         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 4        | 10.87         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 19       | 10.85         |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 10       | 10.85         |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 17       | 10.84         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 11       | 10.84         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 3        | 10.84         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 16       | 10.84         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 12       | 10.83         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 11       | 10.83         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 9        | 10.82         |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 15       | 10.82         |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 9        | 10.81         |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 3        | 10.81         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 16       | 10.8          |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 10       | 10.8          |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 17       | 10.79         |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 17       | 10.79         |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 2        | 10.79         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 20       | 10.78         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 15       | 10.78         |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 5        | 10.77         |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 8        | 10.77         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 13       | 10.77         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 6        | 10.76         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 4        | 10.76         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 4        | 10.75         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 11       | 10.74         |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 7        | 10.74         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 12       | 10.74         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 8        | 10.74         |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 10       | 10.74         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 15       | 10.73         |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 3        | 10.73         |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 7        | 10.73         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 11       | 10.73         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 7        | 10.72         |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 13       | 10.72         |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 3        | 10.71         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 11       | 10.71         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 1        | 10.7          |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 12       | 10.7          |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 18       | 10.69         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 9        | 10.69         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 10       | 10.69         |
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 12       | 10.69         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 9        | 10.68         |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 13       | 10.68         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 3        | 10.67         |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 14       | 10.67         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 20       | 10.66         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 20       | 10.66         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 5        | 10.65         |
| (1,681) | 1:47:A:SER:H  | 1:74:A:SER:CB | 3        | 10.65         |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 11       | 10.65         |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 12       | 10.65         |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 10       | 10.65         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 19       | 10.64         |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 13       | 10.64         |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 12       | 10.63         |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 3        | 10.63         |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 15       | 10.63         |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 16       | 10.63         |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 9        | 10.62         |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 6        | 10.61         |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 4        | 10.6          |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 8        | 10.59         |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 2        | 10.59         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 6        | 10.58         |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 16       | 10.57         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 2        | 10.57         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 3        | 10.57         |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 9        | 10.57         |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 17       | 10.57         |
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 15       | 10.57         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 1        | 10.56         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 20       | 10.56         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 18       | 10.56         |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 19       | 10.56         |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 12       | 10.55         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 18       | 10.54         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 5        | 10.54         |
| (1,660) | 1:46:A:VAL:H  | 1:74:A:SER:CB | 11       | 10.54         |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 7        | 10.54         |
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 14       | 10.54         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 4        | 10.53         |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 6        | 10.52         |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 7        | 10.51         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 4        | 10.51         |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 5        | 10.51         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 19       | 10.51         |
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 14       | 10.51         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 19       | 10.5          |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 5        | 10.49         |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 2        | 10.49         |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 8        | 10.49         |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 13       | 10.49         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 3        | 10.49         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 9        | 10.48         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 4        | 10.48         |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 6        | 10.47         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 18       | 10.47         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 13       | 10.46         |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 17       | 10.45         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 3        | 10.45         |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 15       | 10.45         |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 18       | 10.44         |
| (1,806) | 1:74:A:SER:CB | 1:99:A:LEU:H  | 10       | 10.43         |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 9        | 10.42         |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 18       | 10.42         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 20       | 10.42         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 20       | 10.41         |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 1        | 10.38         |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 5        | 10.38         |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 17       | 10.38         |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 14       | 10.36         |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 4        | 10.36         |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 8        | 10.36         |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 3        | 10.35         |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 14       | 10.35         |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 5        | 10.34         |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 14       | 10.34         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 8        | 10.34         |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 16       | 10.32         |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 10       | 10.32         |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 4        | 10.32         |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 2        | 10.31         |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 2        | 10.31         |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 7        | 10.31         |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 6        | 10.3          |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 15       | 10.3          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 10       | 10.29         |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 12       | 10.29         |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 10       | 10.29         |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 13       | 10.29         |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 17       | 10.28         |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 6        | 10.28         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 8        | 10.27         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 5        | 10.27         |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 9        | 10.26         |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 12       | 10.24         |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 10       | 10.24         |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 17       | 10.23         |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 15       | 10.23         |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 8        | 10.22         |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 9        | 10.22         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 9        | 10.22         |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 13       | 10.22         |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 13       | 10.22         |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 12       | 10.21         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 2        | 10.21         |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 5        | 10.21         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 17       | 10.21         |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 14       | 10.2          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 20       | 10.2          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 8        | 10.2          |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 1        | 10.2          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 13       | 10.19         |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 14       | 10.19         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 11       | 10.19         |
| (1,424) | 1:15:A:GLY:H  | 1:47:A:SER:CB | 11       | 10.18         |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 13       | 10.18         |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 11       | 10.17         |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 1        | 10.16         |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 6        | 10.16         |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 17       | 10.16         |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 10       | 10.16         |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 1        | 10.15         |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 8        | 10.15         |
| (1,418) | 1:14:A:PHE:H  | 1:47:A:SER:CB | 11       | 10.14         |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 2        | 10.13         |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 7        | 10.13         |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 4        | 10.12         |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 7        | 10.12         |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 7        | 10.11         |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 9        | 10.09         |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 18       | 10.09         |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 8        | 10.08         |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 10       | 10.08         |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 3        | 10.08         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 1        | 10.08         |
| (1,346) | 1:3:A:LEU:H   | 1:56:A:SER:CB | 16       | 10.08         |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 16       | 10.07         |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 2        | 10.07         |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 20       | 10.06         |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 11       | 10.04         |
| (1,430) | 1:16:A:SER:H  | 1:47:A:SER:CB | 16       | 10.04         |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 12       | 10.04         |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 7        | 10.03         |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 4        | 10.03         |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 16       | 10.02         |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 15       | 10.02         |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 19       | 10.02         |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 18       | 10.02         |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 12       | 10.01         |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 5        | 10.01         |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 9        | 10.0          |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 20       | 10.0          |
| (1,704) | 1:48:A:ASN:H  | 1:74:A:SER:CB | 2        | 10.0          |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 1        | 10.0          |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 19       | 9.99          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 9        | 9.99          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 13       | 9.99          |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 18       | 9.99          |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 18       | 9.98          |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 3        | 9.98          |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 15       | 9.98          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 8        | 9.97          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 15       | 9.97          |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 10       | 9.96          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 18       | 9.96          |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 14       | 9.96          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 12       | 9.95          |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 14       | 9.95          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 6        | 9.95          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 9        | 9.94          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 4        | 9.94          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 16       | 9.94          |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 6        | 9.94          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 5        | 9.93          |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 8        | 9.93          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 12       | 9.92          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 3        | 9.92          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 12       | 9.92          |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 5        | 9.91          |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 4        | 9.9           |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 18       | 9.9           |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 19       | 9.9           |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 12       | 9.9           |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 6        | 9.89          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 17       | 9.89          |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 18       | 9.88          |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 18       | 9.87          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 17       | 9.87          |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 17       | 9.87          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 19       | 9.86          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 19       | 9.86          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 15       | 9.85          |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 18       | 9.85          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 10       | 9.84          |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 15       | 9.84          |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 3        | 9.84          |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 9        | 9.84          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 7        | 9.83          |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 18       | 9.83          |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 8        | 9.83          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 17       | 9.83          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 2        | 9.83          |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 14       | 9.81          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 1        | 9.81          |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 18       | 9.81          |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 3        | 9.81          |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 8        | 9.8           |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 20       | 9.8           |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 12       | 9.79          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 17       | 9.79          |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 16       | 9.79          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 2        | 9.79          |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 17       | 9.78          |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 19       | 9.78          |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 5        | 9.78          |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 6        | 9.77          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 6        | 9.76          |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 13       | 9.76          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 7        | 9.76          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 8        | 9.75          |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 3        | 9.74          |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 19       | 9.73          |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 4        | 9.73          |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 1        | 9.72          |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 16       | 9.72          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 13       | 9.72          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 14       | 9.72          |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 11       | 9.71          |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 3        | 9.71          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 3        | 9.71          |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 12       | 9.71          |
| (1,381) | 1:8:A:TYR:H   | 1:56:A:SER:CB | 14       | 9.71          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 18       | 9.69          |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 13       | 9.69          |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 8        | 9.68          |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 16       | 9.68          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 19       | 9.67          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 19       | 9.67          |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 7        | 9.66          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 11       | 9.66          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 10       | 9.65          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 11       | 9.64          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 19       | 9.64          |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 7        | 9.64          |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 11       | 9.64          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 12       | 9.63          |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 12       | 9.63          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 9        | 9.63          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 8        | 9.62          |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 6        | 9.62          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 8        | 9.61          |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 13       | 9.61          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 7        | 9.61          |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 1        | 9.6           |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 20       | 9.6           |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 12       | 9.6           |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 1        | 9.6           |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 20       | 9.59          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 7        | 9.59          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 18       | 9.59          |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 12       | 9.58          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 4        | 9.58          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 11       | 9.58          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 15       | 9.58          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 10       | 9.58          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 5        | 9.56          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 6        | 9.56          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 20       | 9.56          |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 4        | 9.56          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 18       | 9.55          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 6        | 9.54          |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 20       | 9.54          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 7        | 9.54          |
| (1,805) | 1:74:A:SER:CB | 1:98:A:LEU:H  | 13       | 9.53          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 15       | 9.53          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 1        | 9.53          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 13       | 9.53          |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 15       | 9.53          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 10       | 9.52          |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 16       | 9.52          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 1        | 9.52          |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 1        | 9.51          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 10       | 9.5           |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 20       | 9.5           |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 7        | 9.49          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 6        | 9.49          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 15       | 9.48          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 13       | 9.48          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 12       | 9.48          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 3        | 9.47          |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 10       | 9.47          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 19       | 9.46          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 3        | 9.45          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 4        | 9.45          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 8        | 9.44          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 4        | 9.44          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 15       | 9.44          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 19       | 9.44          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 3        | 9.44          |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 4        | 9.44          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 17       | 9.43          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 13       | 9.41          |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 20       | 9.41          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 17       | 9.41          |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 1        | 9.41          |
| (1,346) | 1:3:A:LEU:H   | 1:56:A:SER:CB | 14       | 9.41          |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 5        | 9.4           |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 17       | 9.39          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 5        | 9.39          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 10       | 9.38          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 1        | 9.38          |
| (1,367) | 1:6:A:PHE:H   | 1:56:A:SER:CB | 5        | 9.38          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 6        | 9.37          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 1        | 9.37          |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 15       | 9.37          |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 13       | 9.37          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 20       | 9.36          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 1        | 9.36          |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 4        | 9.36          |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 17       | 9.36          |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 5        | 9.35          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 2        | 9.34          |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 20       | 9.34          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 7        | 9.33          |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 10       | 9.33          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 2        | 9.33          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 20       | 9.32          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 7        | 9.3           |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 8        | 9.3           |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 7        | 9.3           |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 10       | 9.29          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 9        | 9.29          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 3        | 9.29          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 11       | 9.29          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 20       | 9.29          |
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 5        | 9.29          |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 2        | 9.28          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 2        | 9.28          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 1        | 9.28          |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 4        | 9.27          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 9        | 9.27          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 1        | 9.26          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 10       | 9.26          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 8        | 9.26          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 20       | 9.26          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 2        | 9.26          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 6        | 9.25          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 18       | 9.25          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 19       | 9.25          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 18       | 9.24          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 11       | 9.24          |
| (1,374) | 1:7:A:GLY:H   | 1:56:A:SER:CB | 13       | 9.23          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 15       | 9.22          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 6        | 9.22          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 5        | 9.22          |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 18       | 9.22          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 14       | 9.21          |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 15       | 9.21          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 5        | 9.2           |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 15       | 9.19          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 19       | 9.19          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 8        | 9.19          |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 5        | 9.19          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 2        | 9.18          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 2        | 9.17          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 19       | 9.17          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 2        | 9.16          |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 3        | 9.16          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 12       | 9.16          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 17       | 9.16          |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 5        | 9.16          |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 1        | 9.14          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 14       | 9.13          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 8        | 9.12          |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 13       | 9.12          |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 14       | 9.12          |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 10       | 9.12          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 1        | 9.11          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 18       | 9.11          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 18       | 9.1           |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 1        | 9.1           |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 5        | 9.1           |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 4        | 9.1           |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 15       | 9.09          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 6        | 9.09          |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 9        | 9.09          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 20       | 9.08          |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 10       | 9.07          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 12       | 9.07          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 9        | 9.04          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 5        | 9.04          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 17       | 9.03          |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 15       | 9.03          |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 11       | 9.03          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 15       | 9.02          |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 18       | 9.02          |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 8        | 9.01          |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 12       | 9.01          |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 20       | 9.01          |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 16       | 9.01          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 17       | 9.01          |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 3        | 9.0           |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 4        | 9.0           |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 5        | 9.0           |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 6        | 9.0           |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 9        | 9.0           |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 10       | 9.0           |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 11       | 9.0           |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 13       | 9.0           |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 15       | 9.0           |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 16       | 9.0           |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 17       | 9.0           |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 18       | 9.0           |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 12       | 9.0           |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 8        | 9.0           |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 13       | 9.0           |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 2        | 9.0           |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 4        | 8.99          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 19       | 8.99          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 18       | 8.99          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 6        | 8.98          |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 7        | 8.97          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 9        | 8.97          |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 2        | 8.96          |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 10       | 8.96          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 15       | 8.95          |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 6        | 8.95          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 4        | 8.95          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 20       | 8.95          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 9        | 8.94          |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 19       | 8.94          |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 5        | 8.94          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 8        | 8.94          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 8        | 8.94          |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 12       | 8.94          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 20       | 8.93          |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 18       | 8.93          |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 4        | 8.93          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 8        | 8.92          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 19       | 8.91          |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 4        | 8.91          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 12       | 8.91          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 18       | 8.91          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 19       | 8.91          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 2        | 8.91          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 9        | 8.9           |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 14       | 8.89          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 2        | 8.89          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 3        | 8.89          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 17       | 8.88          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 13       | 8.88          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 17       | 8.88          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 6        | 8.88          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 16       | 8.87          |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 14       | 8.86          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 3        | 8.86          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 12       | 8.86          |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 16       | 8.86          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 10       | 8.86          |
| (1,353) | 1:4:A:ILE:H   | 1:56:A:SER:CB | 14       | 8.86          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 17       | 8.84          |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 11       | 8.84          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 4        | 8.83          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 10       | 8.82          |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 14       | 8.82          |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 3        | 8.82          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 11       | 8.81          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 4        | 8.81          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 17       | 8.8           |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 18       | 8.8           |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 8        | 8.79          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 7        | 8.79          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 3        | 8.78          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 3        | 8.78          |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 3        | 8.78          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 20       | 8.77          |
| (1,782) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 1        | 8.77          |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 2        | 8.77          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 12       | 8.77          |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 10       | 8.77          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 16       | 8.77          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 7        | 8.76          |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 11       | 8.76          |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 12       | 8.75          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 4        | 8.75          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 15       | 8.75          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 2        | 8.75          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 13       | 8.74          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 18       | 8.74          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 3        | 8.73          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 15       | 8.73          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 16       | 8.73          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 17       | 8.73          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 17       | 8.73          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 9        | 8.73          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 6        | 8.72          |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 8        | 8.72          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 20       | 8.72          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 13       | 8.71          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 13       | 8.71          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 3        | 8.71          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 9        | 8.71          |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 5        | 8.71          |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 7        | 8.69          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 12       | 8.69          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 1        | 8.69          |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 13       | 8.69          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 13       | 8.68          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 9        | 8.68          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 13       | 8.67          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 12       | 8.67          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 2        | 8.67          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 1        | 8.67          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 16       | 8.66          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 7        | 8.66          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 10       | 8.66          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 17       | 8.66          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 11       | 8.65          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 18       | 8.65          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 3        | 8.65          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 6        | 8.65          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 3        | 8.64          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 7        | 8.64          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 10       | 8.63          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 13       | 8.63          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 3        | 8.63          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,340) | 1:2:A:ASP:H   | 1:56:A:SER:CB | 4        | 8.62          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 10       | 8.61          |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 20       | 8.61          |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 14       | 8.61          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 1        | 8.61          |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 19       | 8.6           |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 5        | 8.59          |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 13       | 8.58          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 9        | 8.58          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 4        | 8.57          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 6        | 8.57          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 1        | 8.56          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 14       | 8.56          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 19       | 8.56          |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 11       | 8.55          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 1        | 8.55          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 17       | 8.55          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 17       | 8.55          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 20       | 8.54          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 16       | 8.54          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 4        | 8.54          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 13       | 8.54          |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 14       | 8.53          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 16       | 8.52          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 13       | 8.51          |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 1        | 8.51          |
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 5        | 8.51          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 8        | 8.49          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 6        | 8.49          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 17       | 8.49          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 11       | 8.48          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 10       | 8.48          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 1        | 8.47          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 9        | 8.47          |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 18       | 8.47          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 12       | 8.46          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 7        | 8.46          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 9        | 8.45          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 3        | 8.45          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 7        | 8.45          |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 5        | 8.45          |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 14       | 8.45          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 18       | 8.44          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 19       | 8.44          |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 10       | 8.44          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 2        | 8.44          |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 18       | 8.44          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 6        | 8.43          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 3        | 8.43          |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 10       | 8.43          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 14       | 8.42          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 20       | 8.42          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 14       | 8.42          |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 13       | 8.42          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 2        | 8.41          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 20       | 8.41          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 11       | 8.41          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 16       | 8.4           |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 8        | 8.4           |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 14       | 8.39          |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 7        | 8.39          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 13       | 8.39          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 18       | 8.38          |
| (1,708) | 1:49:A:ASP:H  | 1:74:A:SER:CB | 19       | 8.37          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 8        | 8.37          |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 11       | 8.37          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 20       | 8.36          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 11       | 8.36          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 5        | 8.35          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 8        | 8.35          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 15       | 8.34          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 1        | 8.34          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 6        | 8.34          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 14       | 8.34          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 6        | 8.34          |
| (1,436) | 1:17:A:ILE:H  | 1:47:A:SER:CB | 16       | 8.34          |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 18       | 8.34          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 17       | 8.33          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 17       | 8.33          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 13       | 8.32          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 11       | 8.32          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 4        | 8.31          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 18       | 8.3           |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 7        | 8.3           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 17       | 8.29          |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 3        | 8.29          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 15       | 8.28          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 18       | 8.28          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 13       | 8.27          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 15       | 8.27          |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 5        | 8.27          |
| (1,346) | 1:3:A:LEU:H   | 1:56:A:SER:CB | 5        | 8.27          |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 16       | 8.27          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 6        | 8.26          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 10       | 8.26          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 9        | 8.26          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 7        | 8.26          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 18       | 8.26          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 19       | 8.25          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 6        | 8.25          |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 5        | 8.25          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 18       | 8.25          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 16       | 8.24          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 20       | 8.23          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 17       | 8.22          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 1        | 8.22          |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 4        | 8.21          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 1        | 8.21          |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 19       | 8.2           |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 16       | 8.2           |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 20       | 8.2           |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 10       | 8.19          |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 5        | 8.17          |
| (1,792) | 1:70:A:ARG:H  | 1:99:A:LEU:CB | 11       | 8.16          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 2        | 8.16          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 3        | 8.15          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 8        | 8.15          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 11       | 8.14          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 19       | 8.14          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 6        | 8.13          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 1        | 8.12          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 1        | 8.12          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 16       | 8.12          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 13       | 8.12          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 10       | 8.12          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 12       | 8.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 7        | 8.11          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 11       | 8.11          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 16       | 8.11          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 10       | 8.11          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 20       | 8.1           |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 20       | 8.1           |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 9        | 8.1           |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 18       | 8.1           |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 2        | 8.1           |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 7        | 8.09          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 9        | 8.09          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 15       | 8.09          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 9        | 8.09          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 16       | 8.09          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 7        | 8.08          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 18       | 8.08          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 3        | 8.07          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 10       | 8.06          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 13       | 8.05          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 14       | 8.04          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 14       | 8.04          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 10       | 8.04          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 6        | 8.04          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 18       | 8.03          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 10       | 8.03          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 2        | 8.03          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 17       | 8.03          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 10       | 8.03          |
| (1,375) | 1:7:A:GLY:H   | 1:74:A:SER:CB | 14       | 8.03          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 16       | 8.02          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 12       | 8.02          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 18       | 8.02          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 12       | 8.02          |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 1        | 8.02          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 4        | 8.01          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 10       | 8.01          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 3        | 8.01          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 9        | 8.01          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 11       | 8.01          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 20       | 8.01          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 8        | 8.0           |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 14       | 8.0           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 13       | 8.0           |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 17       | 8.0           |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 4        | 8.0           |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 6        | 8.0           |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 8        | 8.0           |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 15       | 8.0           |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 7        | 8.0           |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 12       | 8.0           |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 13       | 8.0           |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 6        | 8.0           |
| (1,529) | 1:22:A:ARG:H  | 1:47:A:SER:CB | 16       | 8.0           |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 7        | 8.0           |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 8        | 8.0           |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 9        | 8.0           |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 11       | 8.0           |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 14       | 8.0           |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 2        | 8.0           |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 19       | 8.0           |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 5        | 8.0           |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 8        | 8.0           |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 7        | 8.0           |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 10       | 8.0           |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 16       | 8.0           |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 18       | 8.0           |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 3        | 8.0           |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 7        | 8.0           |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 7        | 8.0           |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 10       | 8.0           |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 14       | 8.0           |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 20       | 8.0           |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 16       | 7.99          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 8        | 7.99          |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 9        | 7.99          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 1        | 7.99          |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 17       | 7.99          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 8        | 7.99          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 18       | 7.99          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 16       | 7.98          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 16       | 7.98          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 13       | 7.98          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 16       | 7.98          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 15       | 7.98          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 2        | 7.98          |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 10       | 7.98          |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 16       | 7.98          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 18       | 7.98          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 18       | 7.97          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 17       | 7.97          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 7        | 7.97          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 10       | 7.97          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 17       | 7.97          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 8        | 7.97          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 14       | 7.96          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 1        | 7.96          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 1        | 7.96          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 3        | 7.96          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 12       | 7.96          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 11       | 7.95          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 11       | 7.95          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 11       | 7.95          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 14       | 7.95          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 15       | 7.95          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 9        | 7.94          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 13       | 7.94          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 14       | 7.94          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 14       | 7.94          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 2        | 7.94          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 12       | 7.94          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 16       | 7.94          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 8        | 7.93          |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 5        | 7.92          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 10       | 7.91          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 9        | 7.91          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 7        | 7.9           |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 15       | 7.9           |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 16       | 7.9           |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 13       | 7.9           |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 9        | 7.89          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 5        | 7.89          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 6        | 7.89          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 10       | 7.89          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 13       | 7.89          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 19       | 7.89          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 9        | 7.89          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 10       | 7.88          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 12       | 7.87          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 11       | 7.86          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 9        | 7.86          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 1        | 7.86          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 4        | 7.86          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 11       | 7.86          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 19       | 7.86          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 9        | 7.85          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 2        | 7.85          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 4        | 7.85          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 10       | 7.84          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 16       | 7.84          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 5        | 7.84          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 2        | 7.84          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 7        | 7.84          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 3        | 7.84          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 20       | 7.84          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 7        | 7.84          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 17       | 7.83          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 9        | 7.83          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 17       | 7.83          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 13       | 7.83          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 3        | 7.82          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 2        | 7.82          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 1        | 7.82          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 7        | 7.82          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 20       | 7.82          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 16       | 7.81          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 18       | 7.81          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 20       | 7.81          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 9        | 7.81          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 10       | 7.81          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 10       | 7.81          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 14       | 7.81          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 7        | 7.8           |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 18       | 7.8           |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 19       | 7.8           |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 12       | 7.79          |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 14       | 7.79          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 20       | 7.78          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 11       | 7.78          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 1        | 7.78          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 15       | 7.77          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 17       | 7.77          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 14       | 7.77          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 3        | 7.77          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 10       | 7.77          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 18       | 7.76          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 3        | 7.76          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 8        | 7.76          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 16       | 7.76          |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 10       | 7.76          |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 17       | 7.76          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 19       | 7.75          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 4        | 7.75          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 2        | 7.75          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 3        | 7.75          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 15       | 7.75          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 15       | 7.74          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 6        | 7.74          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 19       | 7.74          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 12       | 7.74          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 8        | 7.74          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 1        | 7.74          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 15       | 7.74          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 8        | 7.73          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 1        | 7.73          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 10       | 7.73          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 17       | 7.73          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 1        | 7.73          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 2        | 7.73          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 19       | 7.73          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 8        | 7.73          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 6        | 7.72          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 18       | 7.72          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 6        | 7.72          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 11       | 7.72          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 2        | 7.72          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 12       | 7.72          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 19       | 7.72          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 16       | 7.72          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 4        | 7.72          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 8        | 7.71          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 7        | 7.71          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 20       | 7.71          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 12       | 7.71          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 12       | 7.71          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 18       | 7.71          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 20       | 7.71          |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 5        | 7.71          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 19       | 7.7           |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 9        | 7.7           |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 7        | 7.7           |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 13       | 7.7           |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 1        | 7.69          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 2        | 7.69          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 15       | 7.69          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 19       | 7.69          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 4        | 7.69          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 11       | 7.69          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 9        | 7.68          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 10       | 7.68          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 4        | 7.68          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 12       | 7.68          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 14       | 7.68          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 5        | 7.67          |
| (1,656) | 1:44:A:TYR:H  | 1:74:A:SER:CB | 5        | 7.67          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 17       | 7.67          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 3        | 7.66          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 12       | 7.66          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 13       | 7.66          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 15       | 7.66          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 5        | 7.66          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 14       | 7.66          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 2        | 7.66          |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 3        | 7.66          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 11       | 7.66          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 20       | 7.65          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 11       | 7.65          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 18       | 7.65          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 18       | 7.64          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 5        | 7.64          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 2        | 7.63          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 1        | 7.63          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 6        | 7.63          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 10       | 7.63          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 5        | 7.63          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 7        | 7.62          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 8        | 7.62          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 4        | 7.62          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 4        | 7.62          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 11       | 7.61          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 4        | 7.61          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 3        | 7.61          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 20       | 7.61          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 10       | 7.61          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 5        | 7.6           |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 20       | 7.6           |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 5        | 7.6           |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 17       | 7.6           |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 5        | 7.6           |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 7        | 7.6           |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 9        | 7.59          |
| (1,682) | 1:47:A:SER:CB | 1:77:A:ILE:H  | 5        | 7.59          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 17       | 7.59          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 16       | 7.59          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 3        | 7.59          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 12       | 7.59          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 12       | 7.58          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 3        | 7.58          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 12       | 7.58          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 3        | 7.58          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 16       | 7.57          |
| (1,365) | 1:6:A:PHE:H   | 1:37:A:CYS:CB | 4        | 7.57          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 12       | 7.56          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 1        | 7.55          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 4        | 7.55          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 13       | 7.55          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 6        | 7.54          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 3        | 7.54          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 4        | 7.54          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 10       | 7.54          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 20       | 7.54          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 1        | 7.54          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 17       | 7.54          |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 3        | 7.54          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 19       | 7.53          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 1        | 7.53          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 20       | 7.53          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 14       | 7.52          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 14       | 7.52          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 17       | 7.52          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 15       | 7.52          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 8        | 7.52          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 8        | 7.51          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 1        | 7.51          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 5        | 7.51          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 12       | 7.51          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 1        | 7.51          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 11       | 7.51          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 3        | 7.51          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 16       | 7.5           |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 7        | 7.5           |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 15       | 7.5           |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 17       | 7.5           |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 5        | 7.5           |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 11       | 7.5           |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 6        | 7.5           |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 8        | 7.5           |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 3        | 7.5           |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 3        | 7.49          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 6        | 7.49          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 11       | 7.49          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 16       | 7.49          |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 4        | 7.49          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 5        | 7.49          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 2        | 7.49          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 1        | 7.49          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 9        | 7.49          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 20       | 7.48          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 10       | 7.48          |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 1        | 7.48          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 6        | 7.47          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 11       | 7.47          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 8        | 7.47          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 15       | 7.46          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 10       | 7.46          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 19       | 7.46          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 4        | 7.46          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 16       | 7.45          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 17       | 7.45          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 18       | 7.45          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 19       | 7.45          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 1        | 7.45          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 12       | 7.45          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 18       | 7.44          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 5        | 7.44          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 2        | 7.44          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 15       | 7.44          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 7        | 7.44          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 20       | 7.44          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 17       | 7.44          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 9        | 7.44          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 6        | 7.43          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 6        | 7.43          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 12       | 7.43          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 7        | 7.43          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 13       | 7.42          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 13       | 7.42          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 6        | 7.42          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 14       | 7.42          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 6        | 7.42          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 12       | 7.42          |
| (1,351) | 1:4:A:ILE:H   | 1:37:A:CYS:CB | 5        | 7.42          |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 3        | 7.42          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 4        | 7.41          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 4        | 7.41          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 10       | 7.41          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 15       | 7.41          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 20       | 7.41          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 6        | 7.4           |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 3        | 7.4           |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 12       | 7.4           |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 17       | 7.4           |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 5        | 7.39          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 16       | 7.39          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 8        | 7.39          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 9        | 7.39          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 18       | 7.39          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 14       | 7.39          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 12       | 7.38          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 17       | 7.38          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 10       | 7.38          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 15       | 7.38          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 13       | 7.38          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 17       | 7.38          |
| (1,443) | 1:18:A:PHE:H  | 1:74:A:SER:CB | 20       | 7.38          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 14       | 7.38          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 1        | 7.37          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 19       | 7.37          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 14       | 7.37          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 16       | 7.37          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 6        | 7.37          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 10       | 7.37          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 7        | 7.36          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 20       | 7.36          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 7        | 7.36          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 18       | 7.36          |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 13       | 7.36          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 16       | 7.35          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 18       | 7.35          |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 19       | 7.35          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 16       | 7.35          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 18       | 7.35          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 10       | 7.35          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 12       | 7.35          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 8        | 7.34          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 17       | 7.34          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 6        | 7.34          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 17       | 7.34          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 20       | 7.34          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 12       | 7.34          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 4        | 7.34          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 7        | 7.33          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 18       | 7.33          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 9        | 7.33          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 2        | 7.33          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 14       | 7.32          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 12       | 7.32          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 11       | 7.32          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 5        | 7.32          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 3        | 7.32          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 13       | 7.31          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 10       | 7.31          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 16       | 7.3           |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 7        | 7.3           |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 11       | 7.3           |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 15       | 7.3           |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 1        | 7.29          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 6        | 7.29          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 8        | 7.29          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 17       | 7.29          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 10       | 7.29          |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 19       | 7.29          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 19       | 7.29          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 19       | 7.29          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 1        | 7.28          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 19       | 7.28          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 14       | 7.28          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 13       | 7.28          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 10       | 7.28          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 4        | 7.28          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 18       | 7.28          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 10       | 7.28          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 2        | 7.28          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 15       | 7.28          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 17       | 7.28          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 6        | 7.28          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 19       | 7.27          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 4        | 7.27          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 18       | 7.27          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 11       | 7.27          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 9        | 7.27          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 1        | 7.27          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 12       | 7.26          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 10       | 7.26          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 4        | 7.25          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 7        | 7.25          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 8        | 7.24          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 11       | 7.24          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 17       | 7.23          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 20       | 7.23          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 2        | 7.23          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 18       | 7.23          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 6        | 7.23          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 13       | 7.23          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 15       | 7.23          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 10       | 7.22          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 12       | 7.22          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 1        | 7.22          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 17       | 7.22          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 12       | 7.22          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 12       | 7.22          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 14       | 7.22          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 20       | 7.22          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 11       | 7.22          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 18       | 7.21          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 8        | 7.21          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 14       | 7.21          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 10       | 7.21          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 18       | 7.21          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 2        | 7.21          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 9        | 7.21          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 6        | 7.2           |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 2        | 7.2           |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 1        | 7.2           |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 19       | 7.2           |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 7        | 7.2           |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 2        | 7.2           |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 11       | 7.2           |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 20       | 7.19          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 12       | 7.19          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 14       | 7.19          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 15       | 7.19          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 18       | 7.19          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 19       | 7.19          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 13       | 7.19          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 13       | 7.18          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 9        | 7.18          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 18       | 7.18          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 18       | 7.18          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 5        | 7.18          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 5        | 7.17          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 19       | 7.17          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 15       | 7.17          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 10       | 7.17          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 11       | 7.17          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 10       | 7.17          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 14       | 7.17          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 13       | 7.17          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 4        | 7.17          |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 15       | 7.17          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 14       | 7.17          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 20       | 7.16          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 9        | 7.16          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 13       | 7.16          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 18       | 7.16          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 18       | 7.16          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 13       | 7.16          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 9        | 7.15          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 20       | 7.15          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 4        | 7.15          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 16       | 7.15          |
| (1,344) | 1:3:A:LEU:H   | 1:37:A:CYS:CB | 5        | 7.15          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 4        | 7.14          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 18       | 7.14          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 18       | 7.14          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 5        | 7.14          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 4        | 7.14          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 8        | 7.14          |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 18       | 7.14          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 5        | 7.14          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 14       | 7.13          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 5        | 7.13          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 9        | 7.13          |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 8        | 7.13          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 16       | 7.13          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 5        | 7.13          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 17       | 7.13          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 15       | 7.13          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 9        | 7.12          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 1        | 7.12          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 6        | 7.11          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 11       | 7.11          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 17       | 7.11          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 11       | 7.11          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 4        | 7.11          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 16       | 7.1           |
| (1,595) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 20       | 7.1           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 1        | 7.1           |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 8        | 7.1           |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 12       | 7.1           |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 12       | 7.09          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 13       | 7.09          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 2        | 7.09          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 16       | 7.09          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 6        | 7.09          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 1        | 7.09          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 13       | 7.08          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 12       | 7.08          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 8        | 7.08          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 3        | 7.08          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 3        | 7.08          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 13       | 7.08          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 8        | 7.08          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 5        | 7.08          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 19       | 7.07          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 10       | 7.07          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 14       | 7.07          |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 15       | 7.07          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 14       | 7.07          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 6        | 7.07          |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 12       | 7.07          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 5        | 7.07          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 18       | 7.07          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 9        | 7.06          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 10       | 7.06          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 19       | 7.06          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 19       | 7.06          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 4        | 7.06          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 17       | 7.06          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 9        | 7.05          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 10       | 7.05          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 5        | 7.05          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 6        | 7.05          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 18       | 7.05          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 5        | 7.05          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 8        | 7.05          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 20       | 7.05          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 3        | 7.05          |
| (1,760) | 1:59:A:THR:H  | 1:74:A:SER:CB | 2        | 7.04          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 1        | 7.04          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 1        | 7.04          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 16       | 7.04          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 2        | 7.04          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 12       | 7.04          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 3        | 7.04          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 8        | 7.04          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 5        | 7.04          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 13       | 7.04          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 4        | 7.03          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 5        | 7.03          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 15       | 7.03          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 18       | 7.03          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 20       | 7.03          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 7        | 7.03          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 5        | 7.03          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 1        | 7.02          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 11       | 7.02          |
| (1,790) | 1:69:A:VAL:H  | 1:99:A:LEU:CB | 14       | 7.02          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 2        | 7.02          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 14       | 7.02          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 1        | 7.02          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 10       | 7.02          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 7        | 7.02          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 6        | 7.02          |
| (1,448) | 1:19:A:GLY:H  | 1:74:A:SER:CB | 14       | 7.02          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 16       | 7.01          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 16       | 7.01          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 15       | 7.01          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 8        | 7.01          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 7        | 7.01          |
| (1,804) | 1:74:A:SER:CB | 1:97:A:LEU:H  | 3        | 7.0           |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 15       | 7.0           |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 17       | 7.0           |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 17       | 7.0           |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 20       | 7.0           |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 10       | 7.0           |
| (1,521) | 1:20:A:TYR:CB | 1:99:A:LEU:H  | 5        | 7.0           |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 1        | 7.0           |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 6        | 7.0           |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 6        | 7.0           |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 19       | 7.0           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 4        | 6.99          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 16       | 6.99          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 9        | 6.99          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 16       | 6.99          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 7        | 6.99          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 11       | 6.99          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 5        | 6.99          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 8        | 6.98          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 17       | 6.98          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 2        | 6.98          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 1        | 6.98          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 19       | 6.98          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 19       | 6.97          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 3        | 6.97          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 18       | 6.97          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 9        | 6.97          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 20       | 6.97          |
| (1,402) | 1:11:A:LEU:H  | 1:56:A:SER:CB | 13       | 6.97          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 9        | 6.97          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 15       | 6.97          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 4        | 6.96          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 5        | 6.96          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 3        | 6.96          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 14       | 6.96          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 16       | 6.96          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 11       | 6.96          |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 13       | 6.96          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 15       | 6.96          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 17       | 6.96          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 19       | 6.96          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 3        | 6.96          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 16       | 6.96          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 7        | 6.95          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 10       | 6.95          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 18       | 6.95          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 3        | 6.95          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 2        | 6.95          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 9        | 6.95          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 3        | 6.95          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 14       | 6.95          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 1        | 6.95          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 17       | 6.95          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 4        | 6.95          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 17       | 6.95          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 19       | 6.94          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 18       | 6.94          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 14       | 6.94          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 14       | 6.94          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 19       | 6.94          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 9        | 6.93          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 7        | 6.93          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 17       | 6.93          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 5        | 6.93          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 13       | 6.93          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 6        | 6.93          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 7        | 6.93          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 18       | 6.93          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 6        | 6.92          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 2        | 6.92          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 9        | 6.92          |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 10       | 6.92          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 15       | 6.92          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 14       | 6.92          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 12       | 6.91          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 12       | 6.91          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 5        | 6.91          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 2        | 6.91          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 5        | 6.9           |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 11       | 6.9           |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 2        | 6.9           |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 19       | 6.89          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 20       | 6.89          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 17       | 6.89          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 13       | 6.89          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 11       | 6.89          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 19       | 6.89          |
| (1,368) | 1:6:A:PHE:H   | 1:74:A:SER:CB | 14       | 6.89          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 12       | 6.88          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 16       | 6.88          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 12       | 6.88          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 2        | 6.88          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 16       | 6.88          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 10       | 6.88          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 10       | 6.88          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 3        | 6.88          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 3        | 6.87          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 17       | 6.87          |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 1        | 6.87          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 5        | 6.86          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 15       | 6.86          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 17       | 6.85          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 19       | 6.85          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 6        | 6.85          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 5        | 6.85          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 9        | 6.85          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 10       | 6.85          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 12       | 6.85          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 15       | 6.84          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 16       | 6.84          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 6        | 6.84          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 9        | 6.84          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 18       | 6.84          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 5        | 6.84          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 20       | 6.84          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 6        | 6.83          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 8        | 6.83          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 11       | 6.83          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 12       | 6.83          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 1        | 6.83          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 8        | 6.83          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 3        | 6.83          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 18       | 6.83          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 11       | 6.83          |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 18       | 6.83          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 1        | 6.82          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 10       | 6.82          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 3        | 6.82          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 8        | 6.82          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 7        | 6.82          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 18       | 6.82          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 1        | 6.81          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 18       | 6.81          |
| (1,757) | 1:57:A:LEU:H  | 1:99:A:LEU:CB | 11       | 6.81          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 2        | 6.81          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 20       | 6.8           |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 13       | 6.8           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 13       | 6.8           |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 5        | 6.8           |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 12       | 6.8           |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 12       | 6.8           |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 13       | 6.8           |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 4        | 6.8           |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 1        | 6.8           |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 13       | 6.79          |
| (1,388) | 1:9:A:ALA:H   | 1:56:A:SER:CB | 14       | 6.79          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 8        | 6.78          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 5        | 6.78          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 2        | 6.78          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 8        | 6.78          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 20       | 6.78          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 19       | 6.78          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 6        | 6.77          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 6        | 6.77          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 17       | 6.77          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 2        | 6.77          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 19       | 6.76          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 19       | 6.76          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 12       | 6.76          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 5        | 6.76          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 5        | 6.76          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 3        | 6.76          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 9        | 6.75          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 6        | 6.75          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 1        | 6.75          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 15       | 6.74          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 4        | 6.74          |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 18       | 6.74          |
| (1,795) | 1:74:A:SER:CB | 1:87:A:SER:H  | 3        | 6.73          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 13       | 6.73          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 7        | 6.73          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 10       | 6.73          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 19       | 6.73          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 7        | 6.73          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 6        | 6.73          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 15       | 6.72          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 18       | 6.72          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 17       | 6.72          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 10       | 6.72          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 3        | 6.72          |
| (1,711) | 1:50:A:LYS:H  | 1:74:A:SER:CB | 1        | 6.71          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 5        | 6.71          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 4        | 6.71          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 6        | 6.71          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 11       | 6.71          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 13       | 6.7           |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 5        | 6.7           |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 14       | 6.7           |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 8        | 6.7           |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 13       | 6.7           |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 10       | 6.69          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 3        | 6.69          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 18       | 6.69          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 7        | 6.69          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 13       | 6.69          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 10       | 6.69          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 20       | 6.68          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 3        | 6.68          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 7        | 6.68          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 5        | 6.68          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 20       | 6.68          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 3        | 6.68          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 3        | 6.68          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 6        | 6.68          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 18       | 6.68          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 19       | 6.68          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 1        | 6.68          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 12       | 6.67          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 13       | 6.67          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 8        | 6.67          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 2        | 6.67          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 5        | 6.67          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 15       | 6.67          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 7        | 6.66          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 4        | 6.66          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 19       | 6.66          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 2        | 6.66          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 8        | 6.66          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 18       | 6.65          |
| (1,683) | 1:47:A:SER:CB | 1:78:A:MET:H  | 12       | 6.65          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 10       | 6.65          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 13       | 6.65          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 19       | 6.65          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 20       | 6.65          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 18       | 6.65          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 6        | 6.65          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 10       | 6.64          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 8        | 6.64          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 13       | 6.64          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 7        | 6.64          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 16       | 6.64          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 5        | 6.64          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 9        | 6.64          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 14       | 6.64          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 20       | 6.63          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 3        | 6.63          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 4        | 6.63          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 6        | 6.63          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 12       | 6.63          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 10       | 6.63          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 4        | 6.63          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 4        | 6.63          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 7        | 6.63          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 9        | 6.63          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 7        | 6.63          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 5        | 6.63          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 19       | 6.62          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 1        | 6.62          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 17       | 6.62          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 16       | 6.62          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 15       | 6.62          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 8        | 6.62          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 20       | 6.62          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 16       | 6.61          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 16       | 6.61          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 20       | 6.61          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 20       | 6.6           |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 3        | 6.6           |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 2        | 6.6           |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 9        | 6.6           |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 3        | 6.6           |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 13       | 6.6           |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 4        | 6.59          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 1        | 6.59          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 18       | 6.59          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 6        | 6.59          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 1        | 6.59          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 16       | 6.59          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 10       | 6.59          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 16       | 6.59          |
| (1,420) | 1:14:A:PHE:H  | 1:74:A:SER:CB | 14       | 6.59          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 13       | 6.59          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 20       | 6.59          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 6        | 6.59          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 7        | 6.58          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 1        | 6.58          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 7        | 6.58          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 20       | 6.58          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 17       | 6.57          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 18       | 6.57          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 15       | 6.57          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 6        | 6.57          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 18       | 6.57          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 9        | 6.57          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 7        | 6.57          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 13       | 6.57          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 7        | 6.56          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 18       | 6.56          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 11       | 6.56          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 14       | 6.56          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 4        | 6.56          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 6        | 6.56          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 10       | 6.56          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 4        | 6.56          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 19       | 6.55          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 9        | 6.55          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 7        | 6.54          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 2        | 6.54          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 7        | 6.54          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 14       | 6.54          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 10       | 6.54          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 14       | 6.53          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 20       | 6.53          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 12       | 6.53          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 2        | 6.52          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 14       | 6.52          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 6        | 6.52          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 7        | 6.52          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 1        | 6.52          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 16       | 6.52          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 14       | 6.52          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 5        | 6.51          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 9        | 6.51          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 7        | 6.51          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 5        | 6.51          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 6        | 6.51          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 14       | 6.5           |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 8        | 6.5           |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 8        | 6.49          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 1        | 6.49          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 3        | 6.49          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 14       | 6.48          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 18       | 6.48          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 6        | 6.48          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 16       | 6.48          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 4        | 6.48          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 7        | 6.48          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 3        | 6.48          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 13       | 6.48          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 12       | 6.48          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 17       | 6.48          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 4        | 6.47          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 7        | 6.47          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 4        | 6.47          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 4        | 6.47          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 12       | 6.47          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 1        | 6.47          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 15       | 6.47          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 1        | 6.46          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 14       | 6.46          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 15       | 6.46          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 10       | 6.46          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 1        | 6.46          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 14       | 6.46          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 4        | 6.46          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 1        | 6.46          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 4        | 6.46          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 18       | 6.45          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 6        | 6.45          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 9        | 6.45          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 10       | 6.45          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 18       | 6.45          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 4        | 6.45          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 16       | 6.45          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 20       | 6.45          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 16       | 6.45          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 2        | 6.44          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 2        | 6.44          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 3        | 6.44          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 6        | 6.44          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 18       | 6.44          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 20       | 6.44          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 4        | 6.43          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 3        | 6.43          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 3        | 6.43          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 13       | 6.43          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 15       | 6.43          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 3        | 6.43          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 5        | 6.43          |
| (1,794) | 1:71:A:PHE:H  | 1:99:A:LEU:CB | 1        | 6.42          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 2        | 6.42          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 7        | 6.42          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 8        | 6.42          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 20       | 6.42          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 13       | 6.42          |
| (1,496) | 1:20:A:TYR:H  | 1:74:A:SER:CB | 14       | 6.42          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 11       | 6.42          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 1        | 6.42          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 19       | 6.42          |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 17       | 6.42          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 12       | 6.41          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 19       | 6.41          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 14       | 6.41          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 9        | 6.41          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 12       | 6.41          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 3        | 6.41          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 11       | 6.41          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 7        | 6.41          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 8        | 6.41          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 12       | 6.41          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 1        | 6.4           |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 16       | 6.4           |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 13       | 6.4           |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 8        | 6.4           |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 14       | 6.4           |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 20       | 6.4           |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 4        | 6.4           |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 20       | 6.4           |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 11       | 6.4           |
| (1,426) | 1:15:A:GLY:H  | 1:74:A:SER:CB | 14       | 6.4           |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 5        | 6.39          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 15       | 6.39          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 3        | 6.39          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 10       | 6.39          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 12       | 6.39          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 19       | 6.38          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 13       | 6.38          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 6        | 6.38          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 19       | 6.38          |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 12       | 6.38          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 1        | 6.38          |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 1        | 6.38          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 7        | 6.37          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 5        | 6.37          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 19       | 6.37          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 5        | 6.37          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 16       | 6.37          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 19       | 6.37          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 11       | 6.37          |
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 5        | 6.37          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 14       | 6.36          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 4        | 6.36          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 17       | 6.36          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 6        | 6.36          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 16       | 6.36          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 6        | 6.36          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 8        | 6.35          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 2        | 6.35          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 16       | 6.35          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 20       | 6.35          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 17       | 6.35          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 14       | 6.34          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 3        | 6.34          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 12       | 6.34          |
| (1,446) | 1:19:A:GLY:H  | 1:47:A:SER:CB | 20       | 6.34          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 2        | 6.33          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 12       | 6.33          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 4        | 6.33          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 15       | 6.33          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 11       | 6.33          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 1        | 6.33          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 13       | 6.33          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 19       | 6.33          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 2        | 6.33          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 19       | 6.33          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 11       | 6.33          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 17       | 6.33          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 5        | 6.33          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 15       | 6.33          |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 12       | 6.33          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 7        | 6.32          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 12       | 6.32          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 20       | 6.32          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 6        | 6.32          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 13       | 6.32          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 18       | 6.32          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 20       | 6.32          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 2        | 6.32          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 2        | 6.32          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 17       | 6.32          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 16       | 6.31          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 13       | 6.31          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 19       | 6.31          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 9        | 6.31          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 14       | 6.31          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 15       | 6.31          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 2        | 6.31          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 20       | 6.31          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 14       | 6.31          |
| (1,379) | 1:8:A:TYR:H   | 1:37:A:CYS:CB | 16       | 6.31          |
| (1,684) | 1:47:A:SER:CB | 1:80:A:ALA:H  | 14       | 6.3           |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 6        | 6.3           |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 4        | 6.3           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 6        | 6.3           |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 8        | 6.3           |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 18       | 6.3           |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 4        | 6.3           |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 5        | 6.3           |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 7        | 6.3           |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 10       | 6.3           |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 15       | 6.3           |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 16       | 6.3           |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 18       | 6.3           |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 19       | 6.3           |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 2        | 6.3           |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 16       | 6.3           |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 8        | 6.3           |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 17       | 6.29          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 19       | 6.29          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 12       | 6.29          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 16       | 6.29          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 12       | 6.29          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 2        | 6.28          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 9        | 6.28          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 6        | 6.28          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 13       | 6.28          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 20       | 6.28          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 12       | 6.28          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 18       | 6.28          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 11       | 6.28          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 1        | 6.28          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 13       | 6.28          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 12       | 6.27          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 16       | 6.27          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 5        | 6.27          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 17       | 6.27          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 18       | 6.27          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 16       | 6.27          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 15       | 6.26          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 20       | 6.26          |
| (1,652) | 1:43:A:ALA:H  | 1:74:A:SER:CB | 11       | 6.26          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 3        | 6.26          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 8        | 6.26          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 17       | 6.26          |
| (1,382) | 1:8:A:TYR:H   | 1:74:A:SER:CB | 14       | 6.26          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 20       | 6.25          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 5        | 6.25          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 18       | 6.25          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 10       | 6.25          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 13       | 6.25          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 17       | 6.25          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 11       | 6.24          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 9        | 6.24          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 11       | 6.24          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 14       | 6.24          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 2        | 6.24          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 17       | 6.24          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 13       | 6.24          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 2        | 6.24          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 1        | 6.24          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 12       | 6.23          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 10       | 6.23          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 12       | 6.23          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 4        | 6.23          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 8        | 6.23          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 3        | 6.23          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 9        | 6.23          |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 20       | 6.23          |
| (1,372) | 1:7:A:GLY:H   | 1:37:A:CYS:CB | 4        | 6.23          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 11       | 6.23          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 17       | 6.22          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 14       | 6.22          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 17       | 6.22          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 2        | 6.22          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 19       | 6.22          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 12       | 6.22          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 8        | 6.22          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 11       | 6.22          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 4        | 6.22          |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 17       | 6.22          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 3        | 6.21          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 7        | 6.21          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 12       | 6.21          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 9        | 6.21          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 17       | 6.21          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 9        | 6.21          |
| (1,788) | 1:68:A:GLY:H  | 1:99:A:LEU:CB | 15       | 6.2           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 17       | 6.2           |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 20       | 6.2           |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 4        | 6.2           |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 7        | 6.2           |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 12       | 6.2           |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 11       | 6.19          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 8        | 6.19          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 19       | 6.19          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 13       | 6.19          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 17       | 6.19          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 12       | 6.19          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 5        | 6.19          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 8        | 6.19          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 3        | 6.19          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 2        | 6.19          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 10       | 6.18          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 13       | 6.18          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 6        | 6.18          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 11       | 6.18          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 5        | 6.17          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 2        | 6.17          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 15       | 6.17          |
| (1,504) | 1:20:A:TYR:CB | 1:83:A:VAL:H  | 14       | 6.17          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 19       | 6.17          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 4        | 6.17          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 11       | 6.16          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 17       | 6.16          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 20       | 6.16          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 20       | 6.16          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 19       | 6.16          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 1        | 6.16          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 18       | 6.16          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 7        | 6.16          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 3        | 6.16          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 4        | 6.15          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 5        | 6.15          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 19       | 6.15          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 6        | 6.15          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 20       | 6.15          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 12       | 6.15          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 20       | 6.15          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 11       | 6.15          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 13       | 6.14          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 15       | 6.14          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 14       | 6.14          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 16       | 6.14          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 4        | 6.14          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 16       | 6.14          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 8        | 6.13          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 2        | 6.13          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 11       | 6.13          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 18       | 6.13          |
| (1,403) | 1:11:A:LEU:H  | 1:74:A:SER:CB | 14       | 6.13          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 7        | 6.13          |
| (1,358) | 1:5:A:GLY:H   | 1:37:A:CYS:CB | 16       | 6.13          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 11       | 6.12          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 14       | 6.12          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 2        | 6.12          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 17       | 6.12          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 17       | 6.12          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 10       | 6.12          |
| (1,807) | 1:77:A:ILE:H  | 1:99:A:LEU:CB | 20       | 6.11          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 1        | 6.11          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 13       | 6.11          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 2        | 6.11          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 17       | 6.11          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 7        | 6.1           |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 13       | 6.1           |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 8        | 6.1           |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 11       | 6.1           |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 10       | 6.1           |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 8        | 6.1           |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 14       | 6.1           |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 12       | 6.1           |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 20       | 6.09          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 3        | 6.09          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 18       | 6.09          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 4        | 6.09          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 9        | 6.09          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 15       | 6.09          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 4        | 6.09          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 13       | 6.09          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 20       | 6.08          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 15       | 6.08          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 3        | 6.08          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 16       | 6.08          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 2        | 6.08          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 10       | 6.08          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 18       | 6.08          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 6        | 6.08          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 20       | 6.08          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 2        | 6.07          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 11       | 6.07          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 1        | 6.07          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 2        | 6.07          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 5        | 6.07          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 13       | 6.07          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 3        | 6.07          |
| (1,754) | 1:56:A:SER:H  | 1:99:A:LEU:CB | 11       | 6.06          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 1        | 6.06          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 3        | 6.06          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 8        | 6.06          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 15       | 6.06          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 17       | 6.06          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 1        | 6.06          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 17       | 6.05          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 16       | 6.05          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 13       | 6.05          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 4        | 6.05          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 19       | 6.04          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 9        | 6.04          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 12       | 6.04          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 15       | 6.04          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 14       | 6.04          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 3        | 6.04          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 12       | 6.04          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 6        | 6.04          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 18       | 6.04          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 1        | 6.04          |
| (1,399) | 1:11:A:LEU:H  | 1:20:A:TYR:CB | 16       | 6.04          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 2        | 6.04          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 16       | 6.03          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 19       | 6.03          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 4        | 6.03          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 11       | 6.03          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 5        | 6.03          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 19       | 6.03          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 15       | 6.02          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 9        | 6.02          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 5        | 6.02          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 17       | 6.02          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 17       | 6.02          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 17       | 6.02          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 3        | 6.02          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 9        | 6.02          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 19       | 6.02          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 6        | 6.02          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 1        | 6.02          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 2        | 6.02          |
| (1,395) | 1:10:A:ALA:H  | 1:56:A:SER:CB | 5        | 6.02          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 12       | 6.01          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 2        | 6.01          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 5        | 6.01          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 9        | 6.01          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 10       | 6.01          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 11       | 6.01          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 14       | 6.01          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 19       | 6.01          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 9        | 6.01          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 9        | 6.01          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 8        | 6.01          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 19       | 6.01          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 12       | 6.01          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 7        | 6.01          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 2        | 6.01          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 10       | 6.01          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 12       | 6.01          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 13       | 6.01          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 20       | 6.01          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 19       | 6.01          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 3        | 6.01          |
| (1,549) | 1:25:A:GLY:H  | 1:99:A:LEU:CB | 3        | 6.01          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 5        | 6.01          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 13       | 6.01          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 14       | 6.01          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 20       | 6.01          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 20       | 6.01          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 14       | 6.0           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 8        | 6.0           |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 18       | 6.0           |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 8        | 6.0           |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 14       | 6.0           |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 10       | 6.0           |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 20       | 6.0           |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 14       | 6.0           |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 3        | 6.0           |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 8        | 6.0           |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 9        | 6.0           |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 15       | 6.0           |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 16       | 6.0           |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 2        | 6.0           |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 9        | 6.0           |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 20       | 6.0           |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 7        | 6.0           |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 13       | 6.0           |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 19       | 6.0           |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 11       | 6.0           |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 19       | 6.0           |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 3        | 6.0           |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 6        | 6.0           |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 18       | 6.0           |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 11       | 6.0           |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 15       | 6.0           |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 17       | 6.0           |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 3        | 6.0           |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 4        | 6.0           |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 5        | 6.0           |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 6        | 6.0           |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 11       | 6.0           |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 12       | 6.0           |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 17       | 6.0           |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 8        | 6.0           |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 9        | 6.0           |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 16       | 6.0           |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 9        | 5.99          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 1        | 5.99          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 3        | 5.99          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 16       | 5.99          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 1        | 5.99          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 3        | 5.99          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 17       | 5.99          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 18       | 5.99          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 5        | 5.99          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 8        | 5.99          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 4        | 5.99          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 7        | 5.99          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 3        | 5.98          |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 15       | 5.98          |
| (1,678) | 1:47:A:SER:CB | 1:70:A:ARG:H  | 7        | 5.98          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 4        | 5.98          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 10       | 5.98          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 9        | 5.98          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 2        | 5.98          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 12       | 5.98          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 9        | 5.98          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 12       | 5.98          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 16       | 5.98          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 10       | 5.98          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 16       | 5.98          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 9        | 5.98          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 5        | 5.98          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 15       | 5.97          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 7        | 5.97          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 13       | 5.97          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 15       | 5.97          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 12       | 5.97          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 17       | 5.97          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 7        | 5.97          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 10       | 5.97          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 20       | 5.97          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 15       | 5.97          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 11       | 5.96          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 12       | 5.96          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 7        | 5.96          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 12       | 5.96          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 13       | 5.96          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 4        | 5.96          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 7        | 5.96          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 4        | 5.95          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 4        | 5.95          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 2        | 5.95          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 9        | 5.95          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 18       | 5.95          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 6        | 5.95          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 6        | 5.95          |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 9        | 5.95          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 18       | 5.95          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 16       | 5.95          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 6        | 5.94          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 7        | 5.94          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 2        | 5.94          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 9        | 5.94          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 6        | 5.94          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 5        | 5.94          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 6        | 5.94          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 17       | 5.94          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 3        | 5.93          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 12       | 5.93          |
| (1,714) | 1:51:A:ARG:H  | 1:74:A:SER:CB | 2        | 5.93          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 14       | 5.93          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 19       | 5.93          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 5        | 5.93          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 7        | 5.93          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 6        | 5.93          |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 2        | 5.93          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 15       | 5.93          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 18       | 5.92          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 10       | 5.92          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 5        | 5.92          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 5        | 5.92          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 17       | 5.92          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 19       | 5.91          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 8        | 5.91          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 3        | 5.91          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 7        | 5.91          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 3        | 5.91          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 6        | 5.91          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 2        | 5.91          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 18       | 5.9           |
| (1,685) | 1:47:A:SER:CB | 1:81:A:GLY:H  | 5        | 5.9           |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 16       | 5.9           |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 19       | 5.9           |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 1        | 5.9           |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 10       | 5.9           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 18       | 5.9           |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 3        | 5.9           |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 2        | 5.9           |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 12       | 5.9           |
| (1,396) | 1:10:A:ALA:H  | 1:74:A:SER:CB | 14       | 5.9           |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 18       | 5.89          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 5        | 5.89          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 6        | 5.89          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 6        | 5.89          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 9        | 5.89          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 17       | 5.89          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 13       | 5.88          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 5        | 5.88          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 19       | 5.88          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 10       | 5.88          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 19       | 5.88          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 13       | 5.88          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 9        | 5.88          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 13       | 5.88          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 10       | 5.87          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 19       | 5.87          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 6        | 5.87          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 17       | 5.87          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 15       | 5.87          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 9        | 5.87          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 13       | 5.87          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 2        | 5.86          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 17       | 5.86          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 9        | 5.86          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 15       | 5.86          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 4        | 5.86          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 7        | 5.86          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 14       | 5.86          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 15       | 5.86          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 10       | 5.86          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 12       | 5.86          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 20       | 5.85          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 9        | 5.85          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 13       | 5.85          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 19       | 5.85          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 13       | 5.85          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 15       | 5.85          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 5        | 5.85          |
| (1,534) | 1:23:A:ARG:H  | 1:47:A:SER:CB | 15       | 5.85          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 18       | 5.85          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 10       | 5.85          |
| (1,501) | 1:20:A:TYR:CB | 1:80:A:ALA:H  | 3        | 5.85          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 20       | 5.85          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 11       | 5.85          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 16       | 5.84          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 13       | 5.84          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 3        | 5.84          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 9        | 5.84          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 16       | 5.84          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 17       | 5.83          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 13       | 5.83          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 20       | 5.83          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 19       | 5.83          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 3        | 5.83          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 13       | 5.83          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 6        | 5.83          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 11       | 5.83          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 7        | 5.83          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 4        | 5.83          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 1        | 5.83          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 5        | 5.83          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 15       | 5.82          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 9        | 5.82          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 16       | 5.82          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 19       | 5.82          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 15       | 5.82          |
| (1,463) | 1:20:A:TYR:CB | 1:43:A:ALA:H  | 19       | 5.82          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 18       | 5.82          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 1        | 5.82          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 6        | 5.82          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 17       | 5.81          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 20       | 5.81          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 19       | 5.81          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 17       | 5.81          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 5        | 5.81          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 9        | 5.81          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 19       | 5.81          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 19       | 5.81          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 8        | 5.81          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 12       | 5.81          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 15       | 5.81          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 15       | 5.81          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 8        | 5.8           |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 4        | 5.8           |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 1        | 5.8           |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 5        | 5.8           |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 2        | 5.8           |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 10       | 5.8           |
| (1,454) | 1:20:A:TYR:CB | 1:32:A:GLY:H  | 14       | 5.8           |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 14       | 5.8           |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 19       | 5.8           |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 15       | 5.79          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 7        | 5.79          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 16       | 5.79          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 11       | 5.79          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 14       | 5.79          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 5        | 5.79          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 8        | 5.79          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 20       | 5.79          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 14       | 5.79          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 4        | 5.79          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 6        | 5.79          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 13       | 5.79          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 3        | 5.78          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 8        | 5.78          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 13       | 5.78          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 16       | 5.78          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 15       | 5.78          |
| (1,456) | 1:20:A:TYR:CB | 1:35:A:VAL:H  | 9        | 5.78          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 4        | 5.78          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 18       | 5.78          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 13       | 5.78          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 18       | 5.78          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 17       | 5.77          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 5        | 5.77          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 8        | 5.77          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 17       | 5.77          |
| (1,729) | 1:56:A:SER:CB | 1:66:A:ILE:H  | 16       | 5.77          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 1        | 5.77          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 11       | 5.77          |
| (1,649) | 1:42:A:GLY:H  | 1:74:A:SER:CB | 16       | 5.77          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 12       | 5.77          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 20       | 5.77          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 16       | 5.77          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 18       | 5.77          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 20       | 5.77          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 3        | 5.77          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 15       | 5.77          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 6        | 5.77          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 11       | 5.76          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 3        | 5.76          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 11       | 5.76          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 1        | 5.76          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 5        | 5.76          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 19       | 5.76          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 7        | 5.76          |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 11       | 5.76          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 11       | 5.76          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 1        | 5.75          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 10       | 5.75          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 20       | 5.75          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 4        | 5.75          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 5        | 5.75          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 9        | 5.75          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 13       | 5.75          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 6        | 5.75          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 9        | 5.75          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 12       | 5.75          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 11       | 5.75          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 15       | 5.75          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 17       | 5.75          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 9        | 5.75          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 10       | 5.75          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 13       | 5.75          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 12       | 5.75          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 12       | 5.74          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 8        | 5.74          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 12       | 5.74          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 11       | 5.74          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 7        | 5.74          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 8        | 5.74          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 7        | 5.74          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 19       | 5.74          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 3        | 5.74          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 18       | 5.74          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 6        | 5.74          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 17       | 5.74          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 15       | 5.74          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 8        | 5.73          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 7        | 5.73          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 4        | 5.73          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 3        | 5.73          |
| (1,510) | 1:20:A:TYR:CB | 1:88:A:LEU:H  | 1        | 5.73          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 14       | 5.72          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 7        | 5.72          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 20       | 5.72          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 9        | 5.72          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 9        | 5.72          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 17       | 5.72          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 17       | 5.72          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 5        | 5.72          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 3        | 5.72          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 17       | 5.72          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 17       | 5.72          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 7        | 5.71          |
| (1,803) | 1:74:A:SER:CB | 1:96:A:LEU:H  | 6        | 5.71          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 6        | 5.71          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 6        | 5.71          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 6        | 5.71          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 9        | 5.71          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 2        | 5.71          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 7        | 5.71          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 5        | 5.71          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 4        | 5.7           |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 4        | 5.7           |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 15       | 5.7           |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 4        | 5.7           |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 7        | 5.7           |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 9        | 5.7           |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 4        | 5.7           |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 11       | 5.69          |
| (1,775) | 1:64:A:ALA:H  | 1:74:A:SER:CB | 19       | 5.69          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 1        | 5.69          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 8        | 5.69          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 14       | 5.69          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 6        | 5.69          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 15       | 5.69          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 10       | 5.69          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 1        | 5.69          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 15       | 5.69          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 17       | 5.69          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 5        | 5.68          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 6        | 5.68          |
| (1,675) | 1:47:A:SER:CB | 1:67:A:MET:H  | 20       | 5.68          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 18       | 5.68          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 12       | 5.68          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 20       | 5.68          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 11       | 5.68          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 14       | 5.68          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 7        | 5.68          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 7        | 5.68          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 15       | 5.68          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 19       | 5.68          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 14       | 5.68          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 17       | 5.67          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 8        | 5.67          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 18       | 5.67          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 9        | 5.67          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 7        | 5.67          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 16       | 5.67          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 17       | 5.67          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 20       | 5.67          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 10       | 5.67          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 6        | 5.67          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 2        | 5.67          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 16       | 5.67          |
| (1,408) | 1:12:A:VAL:H  | 1:56:A:SER:CB | 14       | 5.67          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 10       | 5.67          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 1        | 5.67          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 12       | 5.66          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 9        | 5.66          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 15       | 5.66          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 18       | 5.66          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 17       | 5.66          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 5        | 5.65          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 13       | 5.65          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 9        | 5.65          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 3        | 5.65          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 19       | 5.65          |
| (1,601) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 11       | 5.65          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 15       | 5.65          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 12       | 5.65          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 9        | 5.64          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 3        | 5.64          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 4        | 5.64          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 13       | 5.64          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 5        | 5.64          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 10       | 5.64          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 3        | 5.64          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 18       | 5.64          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 11       | 5.64          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 7        | 5.64          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 5        | 5.64          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 19       | 5.63          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 12       | 5.63          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 11       | 5.63          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 20       | 5.63          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 4        | 5.63          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 7        | 5.63          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 10       | 5.63          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 13       | 5.63          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 3        | 5.63          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 5        | 5.63          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 6        | 5.62          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 6        | 5.62          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 9        | 5.62          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 19       | 5.62          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 14       | 5.62          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 9        | 5.62          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 1        | 5.62          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 17       | 5.62          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 12       | 5.62          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 16       | 5.62          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 15       | 5.62          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 12       | 5.61          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 12       | 5.61          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 13       | 5.61          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 12       | 5.61          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 8        | 5.61          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 14       | 5.61          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 11       | 5.61          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 9        | 5.61          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 19       | 5.61          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 11       | 5.61          |
| (1,457) | 1:20:A:TYR:CB | 1:36:A:GLY:H  | 14       | 5.61          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 10       | 5.61          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 15       | 5.61          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 1        | 5.6           |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 3        | 5.6           |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 2        | 5.6           |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 2        | 5.6           |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 11       | 5.6           |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 1        | 5.6           |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 10       | 5.6           |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 3        | 5.6           |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 10       | 5.6           |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 1        | 5.6           |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 18       | 5.6           |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 13       | 5.6           |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 4        | 5.6           |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 2        | 5.59          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 10       | 5.59          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 18       | 5.59          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 6        | 5.59          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 2        | 5.59          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 14       | 5.59          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 16       | 5.59          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 15       | 5.59          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 20       | 5.59          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 16       | 5.59          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 4        | 5.59          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 6        | 5.59          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 14       | 5.59          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 13       | 5.59          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 10       | 5.59          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 3        | 5.59          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 2        | 5.59          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 2        | 5.58          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 8        | 5.58          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 20       | 5.58          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 7        | 5.58          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 4        | 5.58          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 5        | 5.58          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 3        | 5.58          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 18       | 5.58          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 19       | 5.58          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 9        | 5.57          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 3        | 5.57          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 1        | 5.57          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 11       | 5.57          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 17       | 5.57          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 7        | 5.57          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 7        | 5.57          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 2        | 5.57          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 16       | 5.57          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 12       | 5.57          |
| (1,755) | 1:57:A:LEU:H  | 1:74:A:SER:CB | 2        | 5.56          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 9        | 5.56          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 6        | 5.56          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 12       | 5.56          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 7        | 5.56          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 1        | 5.56          |
| (1,611) | 1:37:A:CYS:CB | 1:65:A:THR:H  | 8        | 5.56          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 15       | 5.56          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 4        | 5.56          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 10       | 5.56          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 3        | 5.56          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 9        | 5.56          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 12       | 5.56          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 15       | 5.56          |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 19       | 5.56          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 7        | 5.56          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 5        | 5.55          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 2        | 5.55          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 11       | 5.55          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 15       | 5.54          |
| (1,680) | 1:47:A:SER:CB | 1:72:A:LYS:H  | 16       | 5.54          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 6        | 5.54          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 4        | 5.54          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 4        | 5.54          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 4        | 5.54          |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 8        | 5.53          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 7        | 5.53          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 5        | 5.53          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 3        | 5.53          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 18       | 5.53          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 16       | 5.53          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 10       | 5.53          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 19       | 5.53          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 12       | 5.53          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 7        | 5.53          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 2        | 5.53          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 16       | 5.52          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 9        | 5.52          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 10       | 5.52          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 14       | 5.52          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 9        | 5.52          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 18       | 5.52          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 4        | 5.51          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 18       | 5.51          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 2        | 5.51          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 7        | 5.51          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 17       | 5.51          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 1        | 5.51          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 9        | 5.51          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 8        | 5.5           |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 13       | 5.5           |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 20       | 5.5           |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 8        | 5.5           |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 1        | 5.5           |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 20       | 5.5           |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 5        | 5.5           |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 16       | 5.5           |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 18       | 5.5           |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 18       | 5.5           |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 13       | 5.5           |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 4        | 5.5           |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 16       | 5.5           |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 8        | 5.49          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 6        | 5.49          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 1        | 5.49          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 11       | 5.49          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 9        | 5.49          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 1        | 5.49          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 16       | 5.49          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 14       | 5.49          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 13       | 5.49          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 12       | 5.49          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 3        | 5.49          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 1        | 5.49          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 16       | 5.49          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 20       | 5.49          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 7        | 5.49          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 3        | 5.49          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 14       | 5.48          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 7        | 5.48          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 3        | 5.48          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 13       | 5.48          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 18       | 5.48          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 9        | 5.48          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 17       | 5.48          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 19       | 5.48          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 17       | 5.47          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 5        | 5.47          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 15       | 5.47          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 8        | 5.47          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 20       | 5.47          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 4        | 5.47          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 2        | 5.47          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 11       | 5.47          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 18       | 5.47          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 11       | 5.47          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 3        | 5.46          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 9        | 5.46          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 5        | 5.46          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 20       | 5.46          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 5        | 5.46          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 16       | 5.46          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 2        | 5.45          |
| (1,772) | 1:63:A:LEU:H  | 1:74:A:SER:CB | 19       | 5.45          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 11       | 5.45          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 9        | 5.45          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 16       | 5.45          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 1        | 5.45          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 11       | 5.45          |
| (1,466) | 1:20:A:TYR:CB | 1:46:A:VAL:H  | 15       | 5.45          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 2        | 5.45          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 17       | 5.45          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 6        | 5.44          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 18       | 5.44          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 2        | 5.44          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 13       | 5.44          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 6        | 5.44          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 7        | 5.44          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 7        | 5.44          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 2        | 5.44          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 2        | 5.44          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 2        | 5.44          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 1        | 5.44          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 11       | 5.44          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 1        | 5.44          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 8        | 5.44          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 18       | 5.44          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 1        | 5.43          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 10       | 5.43          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 7        | 5.43          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 5        | 5.43          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 8        | 5.43          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 11       | 5.43          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 4        | 5.43          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 19       | 5.43          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 20       | 5.43          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 16       | 5.43          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 3        | 5.43          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 13       | 5.43          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 19       | 5.42          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 2        | 5.42          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 14       | 5.42          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 2        | 5.42          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 7        | 5.42          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 14       | 5.42          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 5        | 5.42          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 17       | 5.42          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 8        | 5.42          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 3        | 5.42          |
| (1,392) | 1:10:A:ALA:H  | 1:20:A:TYR:CB | 16       | 5.42          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 7        | 5.42          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 12       | 5.41          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 13       | 5.41          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 20       | 5.41          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 19       | 5.41          |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 19       | 5.41          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 12       | 5.41          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 18       | 5.41          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 16       | 5.41          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 5        | 5.41          |
| (1,491) | 1:20:A:TYR:CB | 1:70:A:ARG:H  | 2        | 5.41          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 14       | 5.41          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 20       | 5.41          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 8        | 5.41          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 10       | 5.41          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 7        | 5.41          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 19       | 5.41          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 8        | 5.41          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 2        | 5.41          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 17       | 5.41          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 16       | 5.4           |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 4        | 5.4           |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 11       | 5.4           |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 3        | 5.4           |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 14       | 5.4           |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 20       | 5.4           |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 14       | 5.4           |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 16       | 5.4           |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 10       | 5.4           |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 7        | 5.4           |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 11       | 5.4           |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 12       | 5.4           |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 19       | 5.4           |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 11       | 5.39          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 6        | 5.39          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 12       | 5.39          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 6        | 5.39          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 12       | 5.39          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 10       | 5.39          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 11       | 5.39          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 10       | 5.38          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 18       | 5.38          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 1        | 5.38          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 5        | 5.38          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 10       | 5.38          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 10       | 5.38          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 18       | 5.38          |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 15       | 5.38          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 5        | 5.37          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 8        | 5.37          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 20       | 5.37          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 1        | 5.37          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 18       | 5.37          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 16       | 5.37          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 10       | 5.37          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 5        | 5.37          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 17       | 5.37          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 19       | 5.37          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 2        | 5.37          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 11       | 5.36          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 17       | 5.36          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 12       | 5.36          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 7        | 5.36          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 12       | 5.36          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 8        | 5.36          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 16       | 5.36          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 3        | 5.36          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 16       | 5.36          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 8        | 5.36          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 9        | 5.36          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 16       | 5.36          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 17       | 5.35          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 20       | 5.35          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 17       | 5.35          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 7        | 5.35          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 5        | 5.35          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 4        | 5.35          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 18       | 5.35          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 15       | 5.34          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 12       | 5.34          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 16       | 5.34          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 17       | 5.34          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 14       | 5.34          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 10       | 5.34          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 17       | 5.34          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 6        | 5.34          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 12       | 5.34          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 1        | 5.34          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 9        | 5.34          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 9        | 5.34          |
| (1,465) | 1:20:A:TYR:CB | 1:45:A:ARG:H  | 19       | 5.34          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 20       | 5.33          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 13       | 5.33          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 9        | 5.33          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 18       | 5.33          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 8        | 5.33          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 2        | 5.33          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 8        | 5.33          |
| (1,524) | 1:21:A:LYS:H  | 1:47:A:SER:CB | 16       | 5.33          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 20       | 5.33          |
| (1,377) | 1:7:A:GLY:H   | 1:99:A:LEU:CB | 11       | 5.33          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 18       | 5.32          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 7        | 5.32          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 7        | 5.32          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 15       | 5.32          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 2        | 5.32          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 4        | 5.32          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 8        | 5.32          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 14       | 5.32          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 8        | 5.32          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 8        | 5.31          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 18       | 5.31          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 15       | 5.31          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 4        | 5.31          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 11       | 5.31          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 20       | 5.31          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 15       | 5.31          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 9        | 5.31          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 17       | 5.31          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 17       | 5.3           |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 10       | 5.3           |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 14       | 5.3           |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 8        | 5.3           |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 12       | 5.3           |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 7        | 5.3           |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 12       | 5.3           |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 17       | 5.3           |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 14       | 5.3           |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 8        | 5.3           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 17       | 5.3           |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 4        | 5.3           |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 15       | 5.3           |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 1        | 5.3           |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 16       | 5.3           |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 8        | 5.29          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 4        | 5.29          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 18       | 5.29          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 1        | 5.29          |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 11       | 5.29          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 1        | 5.28          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 15       | 5.28          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 15       | 5.28          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 9        | 5.28          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 6        | 5.28          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 11       | 5.28          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 9        | 5.28          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 9        | 5.28          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 1        | 5.27          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 2        | 5.27          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 5        | 5.27          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 18       | 5.27          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 8        | 5.27          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 11       | 5.27          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 6        | 5.27          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 5        | 5.27          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 7        | 5.27          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 20       | 5.26          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 8        | 5.26          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 11       | 5.26          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 6        | 5.26          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 5        | 5.26          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 6        | 5.26          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 2        | 5.26          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 10       | 5.26          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 5        | 5.26          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 3        | 5.26          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 1        | 5.26          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 7        | 5.25          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 19       | 5.25          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 17       | 5.25          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 6        | 5.25          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 19       | 5.25          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 10       | 5.25          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 11       | 5.25          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 6        | 5.25          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 8        | 5.25          |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 4        | 5.25          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 5        | 5.25          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 2        | 5.24          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 13       | 5.24          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 17       | 5.24          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 9        | 5.24          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 3        | 5.24          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 14       | 5.24          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 4        | 5.24          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 17       | 5.24          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 13       | 5.24          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 6        | 5.24          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 20       | 5.24          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 10       | 5.23          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 17       | 5.23          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 13       | 5.23          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 10       | 5.23          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 1        | 5.22          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 5        | 5.22          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 6        | 5.22          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 12       | 5.22          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 12       | 5.22          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 9        | 5.22          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 11       | 5.22          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 19       | 5.21          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 14       | 5.21          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 15       | 5.21          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 8        | 5.21          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 2        | 5.21          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 2        | 5.2           |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 3        | 5.2           |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 18       | 5.2           |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 15       | 5.2           |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 2        | 5.2           |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 8        | 5.2           |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 20       | 5.2           |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 10       | 5.2           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 17       | 5.2           |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 13       | 5.2           |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 18       | 5.2           |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 15       | 5.2           |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 4        | 5.2           |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 14       | 5.2           |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 13       | 5.2           |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 6        | 5.2           |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 16       | 5.2           |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 15       | 5.19          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 16       | 5.19          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 20       | 5.19          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 5        | 5.19          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 10       | 5.19          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 17       | 5.19          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 5        | 5.19          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 3        | 5.19          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 16       | 5.19          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 3        | 5.19          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 13       | 5.19          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 2        | 5.19          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 16       | 5.19          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 14       | 5.19          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 1        | 5.19          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 20       | 5.18          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 19       | 5.18          |
| (1,665) | 1:47:A:SER:CB | 1:56:A:SER:H  | 9        | 5.18          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 19       | 5.18          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 2        | 5.18          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 6        | 5.18          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 4        | 5.18          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 14       | 5.18          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 2        | 5.18          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 12       | 5.18          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 10       | 5.18          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 6        | 5.18          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 6        | 5.17          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 15       | 5.17          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 12       | 5.17          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 8        | 5.17          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 19       | 5.17          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 13       | 5.17          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 17       | 5.17          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 6        | 5.17          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 4        | 5.17          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 8        | 5.17          |
| (1,812) | 1:83:A:VAL:H  | 1:99:A:LEU:CB | 10       | 5.16          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 7        | 5.16          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 2        | 5.16          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 16       | 5.16          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 15       | 5.16          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 7        | 5.16          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 8        | 5.16          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 3        | 5.16          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 17       | 5.16          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 13       | 5.15          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 12       | 5.15          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 14       | 5.15          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 14       | 5.15          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 19       | 5.15          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 15       | 5.15          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 13       | 5.15          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 18       | 5.15          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 4        | 5.14          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 6        | 5.14          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 16       | 5.14          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 4        | 5.14          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 14       | 5.14          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 20       | 5.14          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 3        | 5.14          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 13       | 5.14          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 14       | 5.14          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 6        | 5.14          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 6        | 5.14          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 9        | 5.14          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 1        | 5.14          |
| (1,604) | 1:37:A:CYS:CB | 1:58:A:PHE:H  | 11       | 5.14          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 12       | 5.14          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 19       | 5.14          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 5        | 5.14          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 10       | 5.14          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 10       | 5.14          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 19       | 5.14          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 16       | 5.14          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 10       | 5.14          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 13       | 5.14          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 14       | 5.13          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 2        | 5.13          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 4        | 5.13          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 12       | 5.13          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 15       | 5.13          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 2        | 5.13          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 1        | 5.13          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 4        | 5.13          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 18       | 5.13          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 19       | 5.12          |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 15       | 5.12          |
| (1,730) | 1:56:A:SER:CB | 1:67:A:MET:H  | 16       | 5.12          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 5        | 5.12          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 4        | 5.12          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 5        | 5.12          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 9        | 5.12          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 18       | 5.12          |
| (1,508) | 1:20:A:TYR:CB | 1:87:A:SER:H  | 14       | 5.12          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 14       | 5.12          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 9        | 5.12          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 15       | 5.12          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 10       | 5.12          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 13       | 5.11          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 1        | 5.11          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 9        | 5.11          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 12       | 5.11          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 3        | 5.11          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 15       | 5.11          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 1        | 5.11          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 3        | 5.11          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 15       | 5.11          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 6        | 5.11          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 8        | 5.11          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 15       | 5.11          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 7        | 5.11          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 9        | 5.11          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 6        | 5.1           |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 9        | 5.1           |
| (1,785) | 1:67:A:MET:H  | 1:99:A:LEU:CB | 10       | 5.1           |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 13       | 5.1           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 3        | 5.1           |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 20       | 5.1           |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 9        | 5.1           |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 6        | 5.1           |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 11       | 5.1           |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 3        | 5.1           |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 2        | 5.1           |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 8        | 5.1           |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 15       | 5.1           |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 18       | 5.09          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 20       | 5.09          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 15       | 5.09          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 11       | 5.09          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 13       | 5.09          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 10       | 5.09          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 15       | 5.09          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 17       | 5.09          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 10       | 5.09          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 6        | 5.09          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 1        | 5.08          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 14       | 5.08          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 10       | 5.08          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 15       | 5.08          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 20       | 5.08          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 3        | 5.08          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 15       | 5.08          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 9        | 5.08          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 1        | 5.08          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 10       | 5.08          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 12       | 5.08          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 7        | 5.08          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 11       | 5.08          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 7        | 5.07          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 7        | 5.07          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 9        | 5.07          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 2        | 5.07          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 14       | 5.07          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 9        | 5.07          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 19       | 5.07          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 13       | 5.07          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 18       | 5.07          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 2        | 5.06          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 13       | 5.06          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 20       | 5.06          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 18       | 5.06          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 8        | 5.06          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 12       | 5.06          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 5        | 5.06          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 1        | 5.06          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 4        | 5.06          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 18       | 5.06          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 5        | 5.06          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 19       | 5.06          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 1        | 5.05          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 11       | 5.05          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 11       | 5.05          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 15       | 5.05          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 1        | 5.05          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 20       | 5.05          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 17       | 5.05          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 12       | 5.05          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 8        | 5.05          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 12       | 5.05          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 20       | 5.04          |
| (1,728) | 1:56:A:SER:CB | 1:65:A:THR:H  | 11       | 5.04          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 16       | 5.04          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 19       | 5.04          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 8        | 5.04          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 6        | 5.04          |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 9        | 5.04          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 6        | 5.04          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 3        | 5.04          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 16       | 5.03          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 6        | 5.03          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 12       | 5.03          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 19       | 5.03          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 7        | 5.03          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 20       | 5.03          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 5        | 5.02          |
| (1,672) | 1:47:A:SER:CB | 1:64:A:ALA:H  | 16       | 5.02          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 4        | 5.02          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 11       | 5.02          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 16       | 5.02          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 20       | 5.02          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 1        | 5.02          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 20       | 5.02          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 1        | 5.02          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 18       | 5.01          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 10       | 5.01          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 16       | 5.01          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 14       | 5.01          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 14       | 5.01          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 19       | 5.01          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 10       | 5.01          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 2        | 5.01          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 11       | 5.01          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 10       | 5.01          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 7        | 5.01          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 5        | 5.01          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 7        | 5.01          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 4        | 5.01          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 8        | 5.0           |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 13       | 5.0           |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 7        | 5.0           |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 1        | 5.0           |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 5        | 5.0           |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 16       | 5.0           |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 10       | 5.0           |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 7        | 5.0           |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 8        | 5.0           |
| (2,1)   | 1:47:A:SER:CB | 1:55:A:VAL:H  | 9        | 4.99          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 19       | 4.99          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 10       | 4.99          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 11       | 4.99          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 4        | 4.99          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 2        | 4.99          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 6        | 4.99          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 5        | 4.99          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 16       | 4.99          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 1        | 4.99          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 18       | 4.99          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 14       | 4.99          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 13       | 4.99          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 7        | 4.99          |
| (1,539) | 1:24:A:GLY:H  | 1:47:A:SER:CB | 15       | 4.99          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 17       | 4.99          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 1        | 4.99          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 12       | 4.99          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 4        | 4.98          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 8        | 4.98          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 8        | 4.98          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 20       | 4.98          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 18       | 4.98          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 15       | 4.98          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 20       | 4.98          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 13       | 4.98          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 11       | 4.98          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 11       | 4.97          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 14       | 4.97          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 6        | 4.97          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 5        | 4.97          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 6        | 4.97          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 14       | 4.96          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 14       | 4.96          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 17       | 4.96          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 1        | 4.96          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 8        | 4.96          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 5        | 4.96          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 5        | 4.96          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 9        | 4.96          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 6        | 4.96          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 10       | 4.96          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 7        | 4.95          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 3        | 4.95          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 9        | 4.95          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 4        | 4.95          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 18       | 4.95          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 19       | 4.95          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 14       | 4.95          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 2        | 4.95          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 1        | 4.95          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 12       | 4.95          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 12       | 4.94          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 5        | 4.94          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 14       | 4.94          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 12       | 4.94          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 8        | 4.94          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 1        | 4.94          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 20       | 4.94          |
| (1,519) | 1:20:A:TYR:CB | 1:97:A:LEU:H  | 18       | 4.94          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 14       | 4.93          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 12       | 4.93          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 16       | 4.93          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 20       | 4.93          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 17       | 4.93          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 9        | 4.93          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 18       | 4.93          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 17       | 4.93          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 7        | 4.93          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 7        | 4.93          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 16       | 4.92          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 19       | 4.92          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 20       | 4.92          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 12       | 4.92          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 9        | 4.92          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 6        | 4.92          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 17       | 4.92          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 5        | 4.92          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 3        | 4.91          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 18       | 4.91          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 4        | 4.91          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 9        | 4.91          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 8        | 4.91          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 2        | 4.91          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 18       | 4.91          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 18       | 4.91          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 1        | 4.91          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 10       | 4.91          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 13       | 4.91          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 16       | 4.91          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 17       | 4.9           |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 14       | 4.9           |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 14       | 4.9           |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 7        | 4.9           |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 14       | 4.9           |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 16       | 4.9           |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 5        | 4.9           |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 19       | 4.9           |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 13       | 4.9           |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 19       | 4.9           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 20       | 4.89          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 11       | 4.89          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 18       | 4.89          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 2        | 4.89          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 6        | 4.89          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 14       | 4.89          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 9        | 4.89          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 15       | 4.89          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 4        | 4.89          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 14       | 4.89          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 14       | 4.89          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 15       | 4.89          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 6        | 4.89          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 20       | 4.89          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 15       | 4.88          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 15       | 4.88          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 20       | 4.88          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 12       | 4.88          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 8        | 4.88          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 20       | 4.88          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 5        | 4.88          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 11       | 4.88          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 4        | 4.88          |
| (1,566) | 1:30:A:ILE:H  | 1:47:A:SER:CB | 19       | 4.88          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 14       | 4.88          |
| (1,467) | 1:20:A:TYR:H  | 1:47:A:SER:CB | 10       | 4.88          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 12       | 4.88          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 18       | 4.87          |
| (1,777) | 1:64:A:ALA:H  | 1:99:A:LEU:CB | 16       | 4.87          |
| (1,667) | 1:47:A:SER:CB | 1:59:A:THR:H  | 9        | 4.87          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 7        | 4.87          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 9        | 4.87          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 1        | 4.87          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 5        | 4.87          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 7        | 4.87          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 16       | 4.87          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 15       | 4.87          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 3        | 4.87          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 16       | 4.87          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 20       | 4.87          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 12       | 4.87          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 3        | 4.87          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 11       | 4.87          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 14       | 4.86          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 5        | 4.86          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 1        | 4.86          |
| (1,673) | 1:47:A:SER:CB | 1:65:A:THR:H  | 14       | 4.86          |
| (1,576) | 1:32:A:GLY:H  | 1:47:A:SER:CB | 19       | 4.86          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 9        | 4.86          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 1        | 4.86          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 18       | 4.86          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 17       | 4.86          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 13       | 4.86          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 9        | 4.85          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 16       | 4.85          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 10       | 4.85          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 8        | 4.85          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 19       | 4.85          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 1        | 4.85          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 17       | 4.85          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 8        | 4.85          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 10       | 4.85          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 18       | 4.85          |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 16       | 4.85          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 16       | 4.84          |
| (1,659) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 16       | 4.84          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 6        | 4.84          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 7        | 4.84          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 9        | 4.84          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 11       | 4.84          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 13       | 4.84          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 16       | 4.84          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 11       | 4.83          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 1        | 4.83          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 14       | 4.83          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 20       | 4.83          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 11       | 4.83          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 5        | 4.83          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 5        | 4.83          |
| (1,437) | 1:17:A:ILE:H  | 1:56:A:SER:CB | 14       | 4.83          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 1        | 4.83          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 20       | 4.82          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 3        | 4.82          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 10       | 4.82          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 4        | 4.82          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 3        | 4.82          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 15       | 4.82          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 5        | 4.82          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 15       | 4.82          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 18       | 4.82          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 12       | 4.82          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 3        | 4.82          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 18       | 4.82          |
| (1,438) | 1:17:A:ILE:H  | 1:74:A:SER:CB | 14       | 4.82          |
| (1,398) | 1:10:A:ALA:H  | 1:99:A:LEU:CB | 16       | 4.82          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 6        | 4.82          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 20       | 4.82          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 2        | 4.81          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 17       | 4.81          |
| (1,671) | 1:47:A:SER:CB | 1:63:A:LEU:H  | 16       | 4.81          |
| (1,526) | 1:21:A:LYS:H  | 1:74:A:SER:CB | 14       | 4.81          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 1        | 4.81          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 8        | 4.81          |
| (1,391) | 1:9:A:ALA:H   | 1:99:A:LEU:CB | 16       | 4.81          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 4        | 4.81          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 4        | 4.81          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 15       | 4.8           |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 2        | 4.8           |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 20       | 4.8           |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 9        | 4.8           |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 1        | 4.8           |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 1        | 4.8           |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 8        | 4.8           |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 6        | 4.8           |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 11       | 4.8           |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 4        | 4.8           |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 2        | 4.8           |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 4        | 4.8           |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 9        | 4.8           |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 6        | 4.79          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 9        | 4.79          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 15       | 4.79          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 15       | 4.79          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 8        | 4.79          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 6        | 4.79          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 9        | 4.79          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 11       | 4.78          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 19       | 4.78          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 9        | 4.78          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 9        | 4.78          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 18       | 4.78          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 16       | 4.78          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 1        | 4.78          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 18       | 4.78          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 7        | 4.77          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 17       | 4.77          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 7        | 4.77          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 5        | 4.77          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 17       | 4.77          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 20       | 4.77          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 14       | 4.77          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 19       | 4.77          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 2        | 4.77          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 9        | 4.77          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 19       | 4.77          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 16       | 4.77          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 20       | 4.77          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 14       | 4.77          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 2        | 4.77          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 8        | 4.76          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 1        | 4.76          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 5        | 4.76          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 16       | 4.76          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 10       | 4.76          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 9        | 4.76          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 13       | 4.76          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 17       | 4.76          |
| (1,405) | 1:11:A:LEU:H  | 1:99:A:LEU:CB | 11       | 4.76          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 15       | 4.75          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 4        | 4.75          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 20       | 4.75          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 1        | 4.75          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 7        | 4.75          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 11       | 4.75          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 16       | 4.75          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 7        | 4.75          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 12       | 4.74          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 17       | 4.74          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 4        | 4.74          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 11       | 4.74          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 9        | 4.74          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 17       | 4.74          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 5        | 4.74          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 9        | 4.74          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 3        | 4.74          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 16       | 4.74          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 15       | 4.74          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 5        | 4.74          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 9        | 4.73          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 17       | 4.73          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 11       | 4.73          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 13       | 4.73          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 10       | 4.73          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 15       | 4.73          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 17       | 4.72          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 9        | 4.72          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 10       | 4.72          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 19       | 4.72          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 11       | 4.72          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 2        | 4.72          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 11       | 4.72          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 13       | 4.72          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 17       | 4.72          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 5        | 4.72          |
| (1,478) | 1:20:A:TYR:CB | 1:57:A:LEU:H  | 19       | 4.72          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 10       | 4.72          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 9        | 4.72          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 17       | 4.72          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 8        | 4.71          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 1        | 4.71          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 20       | 4.71          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 10       | 4.71          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 7        | 4.71          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 13       | 4.71          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 19       | 4.71          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 13       | 4.71          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 19       | 4.71          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 10       | 4.71          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 19       | 4.71          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 11       | 4.71          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 7        | 4.71          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 19       | 4.71          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 9        | 4.71          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 15       | 4.71          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 3        | 4.71          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 1        | 4.71          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 2        | 4.71          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 20       | 4.71          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 13       | 4.71          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 1        | 4.7           |
| (1,677) | 1:47:A:SER:CB | 1:69:A:VAL:H  | 14       | 4.7           |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 1        | 4.7           |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 19       | 4.7           |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 2        | 4.7           |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 16       | 4.69          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 18       | 4.69          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 10       | 4.69          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 8        | 4.69          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 5        | 4.69          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 6        | 4.69          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 3        | 4.69          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 8        | 4.69          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 17       | 4.69          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 1        | 4.69          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 18       | 4.69          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 18       | 4.68          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 6        | 4.68          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 8        | 4.68          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 13       | 4.68          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 5        | 4.68          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 18       | 4.68          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 15       | 4.68          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 20       | 4.68          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 14       | 4.68          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 17       | 4.68          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 11       | 4.68          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 9        | 4.68          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 12       | 4.68          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 2        | 4.68          |
| (1,802) | 1:74:A:SER:CB | 1:95:A:VAL:H  | 15       | 4.67          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 1        | 4.67          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 18       | 4.67          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 1        | 4.67          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 8        | 4.67          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 6        | 4.67          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 16       | 4.67          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 7        | 4.67          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 13       | 4.67          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 18       | 4.67          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 15       | 4.67          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 16       | 4.67          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 11       | 4.67          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 20       | 4.67          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 2        | 4.66          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 11       | 4.66          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 14       | 4.66          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 8        | 4.66          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 18       | 4.66          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 2        | 4.66          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 10       | 4.66          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 9        | 4.66          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 19       | 4.66          |
| (1,808) | 1:78:A:MET:H  | 1:99:A:LEU:CB | 7        | 4.65          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 2        | 4.65          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 16       | 4.65          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 1        | 4.65          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 5        | 4.65          |
| (1,605) | 1:37:A:CYS:CB | 1:59:A:THR:H  | 17       | 4.65          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 15       | 4.65          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 6        | 4.65          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 13       | 4.65          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 8        | 4.65          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 19       | 4.65          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 3        | 4.64          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 6        | 4.64          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 18       | 4.64          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 14       | 4.64          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 15       | 4.64          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 20       | 4.64          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 6        | 4.64          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 5        | 4.64          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 18       | 4.64          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 12       | 4.64          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 3        | 4.64          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 20       | 4.64          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 2        | 4.64          |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 14       | 4.64          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 12       | 4.63          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 14       | 4.63          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 15       | 4.63          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 1        | 4.63          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 3        | 4.63          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 17       | 4.63          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 2        | 4.62          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 5        | 4.62          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 9        | 4.62          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 17       | 4.62          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 6        | 4.62          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 11       | 4.62          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 12       | 4.62          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 20       | 4.62          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 20       | 4.62          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 20       | 4.62          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 13       | 4.62          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 17       | 4.62          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 8        | 4.62          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 4        | 4.61          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 10       | 4.61          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 19       | 4.61          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 20       | 4.61          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 11       | 4.61          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 5        | 4.61          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 5        | 4.61          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 9        | 4.61          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 8        | 4.61          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 8        | 4.61          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 1        | 4.61          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 9        | 4.61          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 17       | 4.6           |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 15       | 4.6           |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 18       | 4.6           |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 20       | 4.6           |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 8        | 4.6           |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 11       | 4.6           |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 11       | 4.6           |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 4        | 4.6           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 14       | 4.6           |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 4        | 4.59          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 13       | 4.59          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 3        | 4.59          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 6        | 4.59          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 6        | 4.59          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 20       | 4.59          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 4        | 4.59          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 16       | 4.59          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 11       | 4.59          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 20       | 4.59          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 3        | 4.59          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 18       | 4.58          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 14       | 4.58          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 3        | 4.58          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 18       | 4.58          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 12       | 4.58          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 2        | 4.58          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 17       | 4.58          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 13       | 4.58          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 19       | 4.58          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 13       | 4.58          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 13       | 4.58          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 19       | 4.58          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 12       | 4.57          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 19       | 4.57          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 13       | 4.57          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 19       | 4.57          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 4        | 4.57          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 16       | 4.57          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 8        | 4.57          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 13       | 4.56          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 18       | 4.56          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 13       | 4.56          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 13       | 4.56          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 20       | 4.56          |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 19       | 4.56          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 10       | 4.56          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 20       | 4.56          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 17       | 4.56          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 18       | 4.56          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 12       | 4.56          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 18       | 4.56          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 8        | 4.56          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 6        | 4.55          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 19       | 4.55          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 17       | 4.55          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 19       | 4.55          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 15       | 4.55          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 11       | 4.55          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 7        | 4.55          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 14       | 4.55          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 17       | 4.55          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 16       | 4.54          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 20       | 4.54          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 18       | 4.54          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 9        | 4.54          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 2        | 4.54          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 17       | 4.54          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 18       | 4.54          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 4        | 4.53          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 1        | 4.53          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 8        | 4.53          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 7        | 4.53          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 20       | 4.53          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 18       | 4.53          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 8        | 4.53          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 8        | 4.53          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 13       | 4.53          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 4        | 4.53          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 15       | 4.53          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 4        | 4.53          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 12       | 4.53          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 4        | 4.53          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 14       | 4.53          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 15       | 4.53          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 3        | 4.53          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 12       | 4.52          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 15       | 4.52          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 13       | 4.52          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 16       | 4.52          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 1        | 4.52          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 5        | 4.52          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 11       | 4.52          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 4        | 4.52          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 16       | 4.52          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 2        | 4.52          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 19       | 4.51          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 3        | 4.51          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 12       | 4.51          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 1        | 4.51          |
| (1,666) | 1:47:A:SER:CB | 1:58:A:PHE:H  | 9        | 4.51          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 14       | 4.51          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 15       | 4.51          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 3        | 4.51          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 7        | 4.51          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 18       | 4.51          |
| (1,811) | 1:82:A:LEU:H  | 1:99:A:LEU:CB | 10       | 4.5           |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 3        | 4.5           |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 9        | 4.5           |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 16       | 4.5           |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 15       | 4.5           |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 4        | 4.49          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 5        | 4.49          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 19       | 4.49          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 1        | 4.49          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 5        | 4.49          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 6        | 4.49          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 11       | 4.49          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 7        | 4.49          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 19       | 4.49          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 19       | 4.48          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 18       | 4.48          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 4        | 4.48          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 13       | 4.48          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 14       | 4.48          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 14       | 4.48          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 11       | 4.48          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 5        | 4.47          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 13       | 4.47          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 5        | 4.47          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 15       | 4.47          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 17       | 4.47          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 2        | 4.47          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 20       | 4.47          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 20       | 4.47          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 17       | 4.47          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 19       | 4.47          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 18       | 4.47          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 8        | 4.46          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 19       | 4.46          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 5        | 4.46          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 5        | 4.46          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 10       | 4.46          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 7        | 4.46          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 14       | 4.46          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 6        | 4.46          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 20       | 4.46          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 7        | 4.46          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 6        | 4.46          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 16       | 4.46          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 16       | 4.45          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 18       | 4.45          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 11       | 4.45          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 18       | 4.45          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 14       | 4.45          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 8        | 4.45          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 4        | 4.45          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 19       | 4.45          |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 2        | 4.45          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 7        | 4.45          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 20       | 4.45          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 15       | 4.45          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 9        | 4.45          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 17       | 4.44          |
| (1,726) | 1:55:A:VAL:H  | 1:99:A:LEU:CB | 11       | 4.44          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 10       | 4.44          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 3        | 4.44          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 13       | 4.44          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 4        | 4.44          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 8        | 4.44          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 4        | 4.44          |
| (1,522) | 1:20:A:TYR:H  | 1:99:A:LEU:CB | 20       | 4.44          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 7        | 4.44          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 4        | 4.44          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 7        | 4.44          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 6        | 4.44          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 10       | 4.44          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 6        | 4.44          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 9        | 4.43          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 6        | 4.43          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 1        | 4.43          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 16       | 4.43          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 15       | 4.43          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 11       | 4.42          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 12       | 4.42          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 16       | 4.42          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 2        | 4.42          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 10       | 4.42          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 2        | 4.42          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 5        | 4.42          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 6        | 4.42          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 8        | 4.42          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 6        | 4.41          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 5        | 4.41          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 17       | 4.41          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 14       | 4.41          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 5        | 4.4           |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 11       | 4.4           |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 11       | 4.4           |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 12       | 4.4           |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 9        | 4.4           |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 8        | 4.4           |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 5        | 4.4           |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 18       | 4.4           |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 6        | 4.4           |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 20       | 4.4           |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 1        | 4.39          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 15       | 4.39          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 12       | 4.39          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 9        | 4.39          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 2        | 4.39          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 3        | 4.39          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 8        | 4.39          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 14       | 4.39          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 12       | 4.39          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 14       | 4.39          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 20       | 4.39          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 3        | 4.39          |
| (1,361) | 1:5:A:GLY:H   | 1:74:A:SER:CB | 14       | 4.39          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 15       | 4.38          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 15       | 4.38          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 3        | 4.38          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 13       | 4.38          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 17       | 4.38          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 15       | 4.38          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 17       | 4.38          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 11       | 4.38          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 14       | 4.38          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 16       | 4.38          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 17       | 4.38          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 15       | 4.38          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 13       | 4.38          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 1        | 4.38          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 18       | 4.38          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 1        | 4.37          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 11       | 4.37          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 11       | 4.37          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 20       | 4.37          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 18       | 4.37          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 9        | 4.37          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 2        | 4.37          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 4        | 4.37          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 20       | 4.37          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 13       | 4.37          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 15       | 4.37          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 7        | 4.37          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 15       | 4.37          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 11       | 4.36          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 7        | 4.36          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 8        | 4.36          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 12       | 4.36          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 5        | 4.36          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 10       | 4.36          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 20       | 4.36          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 2        | 4.36          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 2        | 4.36          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 6        | 4.35          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 12       | 4.35          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 10       | 4.35          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 6        | 4.35          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 2        | 4.35          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 8        | 4.35          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 9        | 4.35          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 17       | 4.35          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 12       | 4.35          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 14       | 4.35          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 2        | 4.35          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 12       | 4.35          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 4        | 4.35          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 13       | 4.35          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 8        | 4.35          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 8        | 4.34          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 13       | 4.34          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 8        | 4.34          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 8        | 4.34          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 3        | 4.34          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 9        | 4.33          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 6        | 4.33          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 7        | 4.33          |
| (1,669) | 1:47:A:SER:CB | 1:61:A:PHE:H  | 9        | 4.33          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 17       | 4.33          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 18       | 4.33          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 3        | 4.33          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 14       | 4.33          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 15       | 4.32          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 5        | 4.32          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 3        | 4.32          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 16       | 4.32          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 12       | 4.32          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 19       | 4.32          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 1        | 4.32          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 12       | 4.32          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 11       | 4.31          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 10       | 4.31          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 7        | 4.31          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 10       | 4.31          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 18       | 4.31          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 1        | 4.31          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 1        | 4.31          |
| (1,619) | 1:37:A:CYS:CB | 1:81:A:GLY:H  | 4        | 4.31          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 4        | 4.31          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 8        | 4.31          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 13       | 4.31          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 1        | 4.31          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 14       | 4.31          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 5        | 4.31          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 18       | 4.31          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 10       | 4.31          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 15       | 4.31          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 12       | 4.3           |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 6        | 4.3           |
| (1,646) | 1:41:A:TYR:H  | 1:74:A:SER:CB | 5        | 4.3           |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 9        | 4.3           |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 5        | 4.3           |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 7        | 4.3           |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 20       | 4.3           |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 13       | 4.3           |
| (1,411) | 1:12:A:VAL:H  | 1:99:A:LEU:CB | 16       | 4.3           |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 20       | 4.3           |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 20       | 4.29          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 9        | 4.29          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 17       | 4.29          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 6        | 4.29          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 11       | 4.29          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 7        | 4.29          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 8        | 4.29          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 19       | 4.29          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 19       | 4.29          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 5        | 4.29          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 7        | 4.29          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 2        | 4.29          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 8        | 4.29          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 19       | 4.29          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 13       | 4.29          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 19       | 4.28          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 14       | 4.28          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 11       | 4.28          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 5        | 4.28          |
| (1,600) | 1:37:A:CYS:CB | 1:54:A:LYS:H  | 3        | 4.28          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 7        | 4.28          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 14       | 4.28          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 10       | 4.28          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 9        | 4.27          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 2        | 4.27          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 7        | 4.27          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 10       | 4.27          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 2        | 4.27          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 19       | 4.27          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 20       | 4.27          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 8        | 4.27          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 6        | 4.27          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 20       | 4.27          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 1        | 4.27          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 18       | 4.27          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 15       | 4.27          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 16       | 4.27          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 11       | 4.27          |
| (1,432) | 1:16:A:SER:H  | 1:74:A:SER:CB | 14       | 4.27          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 6        | 4.27          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 16       | 4.26          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 1        | 4.26          |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 14       | 4.26          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 15       | 4.26          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 6        | 4.26          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 16       | 4.26          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 16       | 4.26          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 3        | 4.26          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 7        | 4.26          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 6        | 4.26          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 13       | 4.26          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 13       | 4.26          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 17       | 4.26          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 3        | 4.26          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 16       | 4.26          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 18       | 4.26          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 1        | 4.26          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 15       | 4.26          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 20       | 4.26          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 11       | 4.26          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 20       | 4.25          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 19       | 4.25          |
| (1,716) | 1:52:A:ASP:H  | 1:74:A:SER:CB | 5        | 4.25          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 13       | 4.25          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 19       | 4.25          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 10       | 4.25          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 13       | 4.25          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 2        | 4.25          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 1        | 4.25          |
| (1,425) | 1:15:A:GLY:H  | 1:56:A:SER:CB | 20       | 4.25          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 3        | 4.25          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 9        | 4.25          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 11       | 4.25          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 6        | 4.24          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 9        | 4.24          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 20       | 4.24          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 18       | 4.24          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 14       | 4.24          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 20       | 4.24          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 6        | 4.24          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 8        | 4.24          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 7        | 4.24          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 18       | 4.24          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 10       | 4.24          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 15       | 4.24          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 10       | 4.24          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 2        | 4.24          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 1        | 4.24          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 11       | 4.24          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 17       | 4.24          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 12       | 4.24          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 18       | 4.24          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 17       | 4.23          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 13       | 4.23          |
| (1,670) | 1:47:A:SER:CB | 1:62:A:PHE:H  | 9        | 4.23          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 20       | 4.23          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 4        | 4.23          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 2        | 4.23          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 15       | 4.23          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 12       | 4.23          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 19       | 4.23          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 8        | 4.23          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 15       | 4.23          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 19       | 4.23          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 8        | 4.22          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 20       | 4.22          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 11       | 4.22          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 3        | 4.22          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 12       | 4.22          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 19       | 4.22          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 5        | 4.22          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 13       | 4.22          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 14       | 4.22          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 10       | 4.22          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 14       | 4.22          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 13       | 4.22          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 3        | 4.22          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 8        | 4.22          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 4        | 4.22          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 6        | 4.22          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 5        | 4.21          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 18       | 4.21          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 14       | 4.21          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 18       | 4.21          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 16       | 4.21          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 2        | 4.21          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 7        | 4.21          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 16       | 4.21          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 11       | 4.21          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 19       | 4.21          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 5        | 4.21          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 5        | 4.2           |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 13       | 4.2           |
| (1,668) | 1:47:A:SER:CB | 1:60:A:ALA:H  | 9        | 4.2           |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 3        | 4.2           |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 14       | 4.2           |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 9        | 4.2           |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 8        | 4.2           |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 6        | 4.2           |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 6        | 4.2           |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 1        | 4.2           |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 20       | 4.2           |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 14       | 4.2           |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 7        | 4.2           |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 15       | 4.19          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 11       | 4.19          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 7        | 4.19          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 1        | 4.19          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 7        | 4.19          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 4        | 4.19          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 9        | 4.19          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 17       | 4.19          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 12       | 4.19          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 11       | 4.19          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 12       | 4.19          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 17       | 4.19          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 3        | 4.19          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 3        | 4.19          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 11       | 4.19          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 17       | 4.19          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 2        | 4.18          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 4        | 4.18          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 11       | 4.18          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 17       | 4.18          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 4        | 4.18          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 4        | 4.18          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 17       | 4.18          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 6        | 4.18          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 5        | 4.18          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 9        | 4.18          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 4        | 4.18          |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 12       | 4.18          |
| (1,734) | 1:56:A:SER:H  | 1:74:A:SER:CB | 2        | 4.17          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 12       | 4.17          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 8        | 4.17          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 7        | 4.17          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 12       | 4.17          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 18       | 4.17          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 17       | 4.17          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 17       | 4.17          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 4        | 4.16          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 14       | 4.16          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 2        | 4.16          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 9        | 4.16          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 7        | 4.16          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 12       | 4.16          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 19       | 4.16          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 16       | 4.16          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 9        | 4.16          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 6        | 4.16          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 9        | 4.15          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 15       | 4.15          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 1        | 4.15          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 12       | 4.15          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 12       | 4.15          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 17       | 4.15          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 4        | 4.15          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 5        | 4.15          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 11       | 4.15          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 6        | 4.15          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 9        | 4.15          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 10       | 4.15          |
| (1,389) | 1:9:A:ALA:H   | 1:74:A:SER:CB | 14       | 4.15          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 10       | 4.15          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 20       | 4.15          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 19       | 4.14          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 15       | 4.14          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 4        | 4.14          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 14       | 4.14          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 4        | 4.14          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 20       | 4.14          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 8        | 4.13          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 10       | 4.13          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 8        | 4.13          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 8        | 4.13          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 4        | 4.13          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 1        | 4.13          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 13       | 4.13          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 10       | 4.13          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 7        | 4.12          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 3        | 4.12          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 3        | 4.12          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 20       | 4.12          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 14       | 4.12          |
| (1,509) | 1:20:A:TYR:H  | 1:87:A:SER:CB | 20       | 4.12          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 3        | 4.12          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 8        | 4.12          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 5        | 4.11          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 11       | 4.11          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 7        | 4.11          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 7        | 4.11          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 1        | 4.1           |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 18       | 4.1           |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 13       | 4.1           |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 2        | 4.1           |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 3        | 4.1           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 2        | 4.1           |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 5        | 4.1           |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 18       | 4.09          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 3        | 4.09          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 16       | 4.09          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 15       | 4.09          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 8        | 4.09          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 11       | 4.09          |
| (1,447) | 1:19:A:GLY:H  | 1:56:A:SER:CB | 20       | 4.09          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 19       | 4.09          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 9        | 4.09          |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 4        | 4.09          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 7        | 4.08          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 4        | 4.08          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 13       | 4.08          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 17       | 4.08          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 14       | 4.08          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 17       | 4.08          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 17       | 4.08          |
| (1,497) | 1:20:A:TYR:CB | 1:75:A:LYS:H  | 10       | 4.08          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 7        | 4.08          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 1        | 4.07          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 18       | 4.07          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 11       | 4.07          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 16       | 4.07          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 15       | 4.07          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 3        | 4.07          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 16       | 4.07          |
| (1,469) | 1:20:A:TYR:CB | 1:49:A:ASP:H  | 15       | 4.07          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 7        | 4.07          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 19       | 4.07          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 16       | 4.07          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 20       | 4.07          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 17       | 4.07          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 17       | 4.06          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 17       | 4.06          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 16       | 4.06          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 3        | 4.06          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 2        | 4.06          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 8        | 4.06          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 15       | 4.06          |
| (1,451) | 1:20:A:TYR:CB | 1:29:A:LEU:H  | 12       | 4.06          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 18       | 4.06          |
| (1,338) | 1:2:A:ASP:H   | 1:37:A:CYS:CB | 4        | 4.06          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 14       | 4.05          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 20       | 4.05          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 14       | 4.05          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 18       | 4.05          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 14       | 4.05          |
| (1,610) | 1:37:A:CYS:CB | 1:64:A:ALA:H  | 15       | 4.05          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 20       | 4.05          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 19       | 4.05          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 7        | 4.05          |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 9        | 4.05          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 1        | 4.05          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 13       | 4.05          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 9        | 4.05          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 2        | 4.04          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 18       | 4.04          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 16       | 4.04          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 12       | 4.04          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 11       | 4.04          |
| (1,620) | 1:37:A:CYS:CB | 1:82:A:LEU:H  | 3        | 4.04          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 18       | 4.04          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 4        | 4.04          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 3        | 4.04          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 7        | 4.04          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 1        | 4.04          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 20       | 4.04          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 8        | 4.04          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 7        | 4.04          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 7        | 4.03          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 13       | 4.03          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 16       | 4.03          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 3        | 4.03          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 20       | 4.03          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 10       | 4.03          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 9        | 4.03          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 8        | 4.03          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 11       | 4.03          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 15       | 4.03          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 15       | 4.03          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 11       | 4.03          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 6        | 4.03          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 5        | 4.03          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 3        | 4.02          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 12       | 4.02          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 17       | 4.02          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 13       | 4.02          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 13       | 4.02          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 8        | 4.02          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 15       | 4.02          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 1        | 4.02          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 14       | 4.02          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 9        | 4.02          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 20       | 4.02          |
| (1,409) | 1:12:A:VAL:H  | 1:74:A:SER:CB | 14       | 4.02          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 12       | 4.01          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 3        | 4.01          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 11       | 4.01          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 19       | 4.01          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 13       | 4.01          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 5        | 4.01          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 3        | 4.01          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 13       | 4.01          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 17       | 4.01          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 18       | 4.01          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 10       | 4.01          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 9        | 4.01          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 17       | 4.01          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 16       | 4.0           |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 2        | 4.0           |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 3        | 4.0           |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 12       | 4.0           |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 18       | 4.0           |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 10       | 4.0           |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 10       | 4.0           |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 18       | 4.0           |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 6        | 4.0           |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 11       | 4.0           |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 10       | 4.0           |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 9        | 4.0           |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 14       | 4.0           |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 3        | 4.0           |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 12       | 4.0           |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 1        | 4.0           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 8        | 3.99          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 4        | 3.99          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 4        | 3.99          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 3        | 3.99          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 14       | 3.99          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 9        | 3.99          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 2        | 3.99          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 12       | 3.98          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 11       | 3.98          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 3        | 3.98          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 6        | 3.98          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 5        | 3.98          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 10       | 3.98          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 2        | 3.98          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 5        | 3.97          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 13       | 3.97          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 11       | 3.97          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 19       | 3.97          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 13       | 3.97          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 8        | 3.97          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 12       | 3.97          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 15       | 3.97          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 10       | 3.97          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 18       | 3.97          |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 14       | 3.97          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 9        | 3.96          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 5        | 3.96          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 3        | 3.96          |
| (1,570) | 1:30:A:ILE:H  | 1:99:A:LEU:CB | 6        | 3.96          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 4        | 3.96          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 6        | 3.96          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 10       | 3.95          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 8        | 3.95          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 5        | 3.95          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 12       | 3.95          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 20       | 3.95          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 17       | 3.95          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 1        | 3.95          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 7        | 3.95          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 10       | 3.95          |
| (1,495) | 1:20:A:TYR:CB | 1:74:A:SER:H  | 12       | 3.95          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 7        | 3.95          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 10       | 3.95          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 1        | 3.94          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 13       | 3.94          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 11       | 3.94          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 3        | 3.94          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 19       | 3.94          |
| (1,584) | 1:35:A:VAL:H  | 1:47:A:SER:CB | 19       | 3.94          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 9        | 3.94          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 12       | 3.94          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 11       | 3.94          |
| (1,385) | 1:9:A:ALA:H   | 1:20:A:TYR:CB | 16       | 3.94          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 17       | 3.93          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 1        | 3.93          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 6        | 3.93          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 2        | 3.93          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 9        | 3.93          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 7        | 3.93          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 10       | 3.93          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 13       | 3.93          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 6        | 3.93          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 14       | 3.93          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 18       | 3.93          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 18       | 3.93          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 10       | 3.93          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 11       | 3.93          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 20       | 3.92          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 5        | 3.92          |
| (1,703) | 1:47:A:SER:CB | 1:99:A:LEU:H  | 4        | 3.92          |
| (1,702) | 1:47:A:SER:CB | 1:98:A:LEU:H  | 4        | 3.92          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 11       | 3.92          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 9        | 3.92          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 2        | 3.92          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 17       | 3.92          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 6        | 3.92          |
| (1,589) | 1:36:A:GLY:H  | 1:47:A:SER:CB | 20       | 3.92          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 12       | 3.92          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 16       | 3.92          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 16       | 3.92          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 10       | 3.92          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 1        | 3.92          |
| (1,810) | 1:81:A:GLY:H  | 1:99:A:LEU:CB | 10       | 3.91          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 6        | 3.91          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 17       | 3.91          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 2        | 3.91          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 1        | 3.91          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 10       | 3.91          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 11       | 3.91          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 2        | 3.91          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 16       | 3.91          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 19       | 3.91          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 2        | 3.91          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 16       | 3.9           |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 15       | 3.9           |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 5        | 3.9           |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 3        | 3.9           |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 5        | 3.9           |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 3        | 3.9           |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 5        | 3.9           |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 13       | 3.9           |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 8        | 3.9           |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 20       | 3.9           |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 1        | 3.89          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 2        | 3.89          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 7        | 3.89          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 5        | 3.89          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 2        | 3.89          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 10       | 3.89          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 11       | 3.89          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 18       | 3.89          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 10       | 3.89          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 1        | 3.89          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 2        | 3.89          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 16       | 3.89          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 15       | 3.89          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 19       | 3.89          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 9        | 3.89          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 3        | 3.88          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 16       | 3.88          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 4        | 3.88          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 16       | 3.88          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 19       | 3.88          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 18       | 3.88          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 15       | 3.88          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 5        | 3.88          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 5        | 3.88          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 10       | 3.88          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 12       | 3.88          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 1        | 3.88          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 16       | 3.88          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 9        | 3.87          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 17       | 3.87          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 8        | 3.87          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 9        | 3.87          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 7        | 3.87          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 5        | 3.87          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 11       | 3.87          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 9        | 3.86          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 4        | 3.86          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 18       | 3.86          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 19       | 3.86          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 18       | 3.86          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 15       | 3.86          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 7        | 3.86          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 3        | 3.86          |
| (1,551) | 1:26:A:VAL:H  | 1:47:A:SER:CB | 20       | 3.86          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 17       | 3.86          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 10       | 3.86          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 7        | 3.85          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 19       | 3.85          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 11       | 3.85          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 15       | 3.85          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 17       | 3.85          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 7        | 3.85          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 13       | 3.85          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 4        | 3.85          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 17       | 3.85          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 15       | 3.85          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 11       | 3.85          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 5        | 3.85          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 20       | 3.85          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 20       | 3.85          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 7        | 3.85          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 3        | 3.85          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 11       | 3.85          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 4        | 3.85          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 12       | 3.85          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 4        | 3.85          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 14       | 3.85          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 7        | 3.84          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 15       | 3.84          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 19       | 3.84          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 4        | 3.84          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 16       | 3.84          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 20       | 3.84          |
| (1,486) | 1:20:A:TYR:CB | 1:65:A:THR:H  | 2        | 3.84          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 5        | 3.84          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 3        | 3.83          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 19       | 3.83          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 20       | 3.83          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 5        | 3.83          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 4        | 3.83          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 6        | 3.83          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 9        | 3.83          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 1        | 3.83          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 20       | 3.83          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 15       | 3.83          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 3        | 3.83          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 12       | 3.83          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 6        | 3.83          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 18       | 3.82          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 16       | 3.82          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 6        | 3.82          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 10       | 3.82          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 8        | 3.82          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 1        | 3.82          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 17       | 3.82          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 14       | 3.82          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 18       | 3.81          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 3        | 3.81          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 4        | 3.81          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 4        | 3.81          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 20       | 3.81          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 5        | 3.81          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 3        | 3.81          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 20       | 3.81          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 19       | 3.81          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 1        | 3.81          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 14       | 3.81          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 12       | 3.81          |
| (1,759) | 1:58:A:PHE:H  | 1:99:A:LEU:CB | 11       | 3.8           |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 5        | 3.8           |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 13       | 3.8           |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 8        | 3.8           |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 8        | 3.8           |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 15       | 3.8           |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 17       | 3.8           |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 10       | 3.79          |
| (1,824) | 1:92:A:LEU:H  | 1:99:A:LEU:CB | 20       | 3.79          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 4        | 3.79          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 5        | 3.79          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 4        | 3.79          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 6        | 3.79          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 14       | 3.79          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 5        | 3.79          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 17       | 3.79          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 2        | 3.79          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 17       | 3.79          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 15       | 3.79          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 9        | 3.79          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 20       | 3.79          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 10       | 3.79          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 7        | 3.79          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 4        | 3.79          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 9        | 3.79          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 19       | 3.79          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 13       | 3.78          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 20       | 3.78          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 16       | 3.78          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 8        | 3.78          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 4        | 3.78          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 17       | 3.78          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 1        | 3.78          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 10       | 3.78          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 8        | 3.78          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 15       | 3.78          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 17       | 3.78          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 9        | 3.78          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 6        | 3.77          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 3        | 3.77          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 16       | 3.77          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 17       | 3.77          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 10       | 3.77          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 15       | 3.77          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 12       | 3.77          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 10       | 3.77          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 14       | 3.77          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 3        | 3.77          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 3        | 3.77          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 17       | 3.77          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 2        | 3.76          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 9        | 3.76          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 7        | 3.76          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 7        | 3.76          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 13       | 3.76          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 15       | 3.76          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 10       | 3.76          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 16       | 3.76          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 8        | 3.76          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 20       | 3.76          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 5        | 3.76          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 6        | 3.76          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 18       | 3.75          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 1        | 3.75          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 1        | 3.75          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 9        | 3.75          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 17       | 3.75          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 6        | 3.75          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 12       | 3.75          |
| (1,475) | 1:20:A:TYR:CB | 1:55:A:VAL:H  | 1        | 3.75          |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 5        | 3.75          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 8        | 3.75          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 18       | 3.74          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 2        | 3.74          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 1        | 3.74          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 12       | 3.74          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 19       | 3.74          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 16       | 3.74          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 11       | 3.74          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 18       | 3.74          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 2        | 3.74          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 1        | 3.74          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 9        | 3.73          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 12       | 3.73          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 15       | 3.73          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 1        | 3.73          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 7        | 3.73          |
| (1,468) | 1:20:A:TYR:CB | 1:48:A:ASN:H  | 19       | 3.73          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 9        | 3.73          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 4        | 3.73          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 16       | 3.72          |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 8        | 3.72          |
| (1,622) | 1:37:A:CYS:CB | 1:84:A:ALA:H  | 20       | 3.72          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 15       | 3.72          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 9        | 3.72          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 19       | 3.72          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 2        | 3.72          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 2        | 3.72          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 10       | 3.72          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 14       | 3.72          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 7        | 3.71          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 10       | 3.71          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 1        | 3.71          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 17       | 3.71          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 11       | 3.71          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 9        | 3.71          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 13       | 3.71          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 12       | 3.71          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 12       | 3.71          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 12       | 3.71          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 6        | 3.71          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 5        | 3.71          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 6        | 3.71          |
| (1,370) | 1:6:A:PHE:H   | 1:99:A:LEU:CB | 16       | 3.71          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 7        | 3.7           |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 14       | 3.7           |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 5        | 3.7           |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 14       | 3.7           |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 1        | 3.7           |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 1        | 3.7           |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 10       | 3.7           |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 20       | 3.7           |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 1        | 3.7           |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 6        | 3.7           |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 9        | 3.7           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 2        | 3.7           |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 12       | 3.7           |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 17       | 3.7           |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 15       | 3.7           |
| (1,474) | 1:20:A:TYR:CB | 1:54:A:LYS:H  | 19       | 3.7           |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 18       | 3.69          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 8        | 3.69          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 6        | 3.69          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 16       | 3.69          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 10       | 3.69          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 8        | 3.69          |
| (1,560) | 1:29:A:LEU:H  | 1:37:A:CYS:CB | 19       | 3.69          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 12       | 3.69          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 19       | 3.69          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 12       | 3.69          |
| (1,414) | 1:13:A:THR:H  | 1:74:A:SER:CB | 14       | 3.69          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 7        | 3.69          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 19       | 3.68          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 8        | 3.68          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 1        | 3.68          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 13       | 3.68          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 6        | 3.68          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 13       | 3.68          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 14       | 3.68          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 17       | 3.68          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 10       | 3.68          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 14       | 3.68          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 8        | 3.67          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 3        | 3.67          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 6        | 3.67          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 15       | 3.67          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 8        | 3.67          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 18       | 3.67          |
| (1,594) | 1:37:A:CYS:CB | 1:47:A:SER:H  | 2        | 3.67          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 8        | 3.67          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 19       | 3.67          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 18       | 3.67          |
| (1,492) | 1:20:A:TYR:CB | 1:71:A:PHE:H  | 12       | 3.67          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 6        | 3.67          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 8        | 3.67          |
| (1,386) | 1:9:A:ALA:H   | 1:37:A:CYS:CB | 16       | 3.67          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 14       | 3.66          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 17       | 3.66          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 15       | 3.66          |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 20       | 3.66          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 6        | 3.66          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 7        | 3.66          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 20       | 3.66          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 16       | 3.66          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 18       | 3.66          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 1        | 3.66          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 6        | 3.66          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 6        | 3.65          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 2        | 3.65          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 6        | 3.65          |
| (1,545) | 1:25:A:GLY:H  | 1:47:A:SER:CB | 15       | 3.65          |
| (1,537) | 1:23:A:ARG:H  | 1:87:A:SER:CB | 20       | 3.65          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 20       | 3.65          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 16       | 3.65          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 11       | 3.65          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 11       | 3.65          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 8        | 3.64          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 2        | 3.64          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 3        | 3.64          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 5        | 3.64          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 8        | 3.64          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 17       | 3.64          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 7        | 3.64          |
| (1,455) | 1:20:A:TYR:CB | 1:33:A:LEU:H  | 14       | 3.64          |
| (1,453) | 1:20:A:TYR:CB | 1:31:A:ALA:H  | 14       | 3.64          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 11       | 3.64          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 1        | 3.63          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 4        | 3.63          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 17       | 3.63          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 3        | 3.63          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 6        | 3.63          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 17       | 3.63          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 19       | 3.63          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 2        | 3.63          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 19       | 3.63          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 14       | 3.63          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 7        | 3.63          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 4        | 3.63          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 8        | 3.62          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 2        | 3.62          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 19       | 3.62          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 17       | 3.62          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 18       | 3.62          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 18       | 3.62          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 19       | 3.62          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 6        | 3.62          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 8        | 3.62          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 9        | 3.62          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 1        | 3.62          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 11       | 3.62          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 15       | 3.62          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 18       | 3.62          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 17       | 3.61          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 17       | 3.61          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 7        | 3.61          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 20       | 3.61          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 14       | 3.61          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 7        | 3.61          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 19       | 3.61          |
| (1,614) | 1:37:A:CYS:CB | 1:68:A:GLY:H  | 2        | 3.61          |
| (1,543) | 1:24:A:GLY:H  | 1:99:A:LEU:CB | 3        | 3.61          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 20       | 3.61          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 2        | 3.6           |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 10       | 3.6           |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 11       | 3.6           |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 16       | 3.6           |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 8        | 3.6           |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 13       | 3.6           |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 19       | 3.6           |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 14       | 3.6           |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 1        | 3.6           |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 18       | 3.6           |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 7        | 3.6           |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 4        | 3.6           |
| (1,623) | 1:37:A:CYS:CB | 1:85:A:GLY:H  | 4        | 3.6           |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 14       | 3.6           |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 2        | 3.6           |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 7        | 3.6           |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 19       | 3.6           |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 17       | 3.6           |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 14       | 3.6           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 7        | 3.6           |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 19       | 3.6           |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 18       | 3.6           |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 5        | 3.59          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 12       | 3.59          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 9        | 3.59          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 20       | 3.59          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 11       | 3.59          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 15       | 3.59          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 10       | 3.59          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 20       | 3.59          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 15       | 3.59          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 7        | 3.59          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 3        | 3.59          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 15       | 3.59          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 18       | 3.58          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 2        | 3.58          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 17       | 3.58          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 3        | 3.58          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 9        | 3.58          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 16       | 3.58          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 20       | 3.57          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 16       | 3.57          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 15       | 3.57          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 18       | 3.57          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 4        | 3.57          |
| (1,613) | 1:37:A:CYS:CB | 1:67:A:MET:H  | 7        | 3.57          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 4        | 3.57          |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 3        | 3.57          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 11       | 3.57          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 4        | 3.57          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 1        | 3.57          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 6        | 3.57          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 18       | 3.56          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 15       | 3.56          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 12       | 3.56          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 17       | 3.56          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 5        | 3.56          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 5        | 3.56          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 15       | 3.56          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 8        | 3.56          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 16       | 3.56          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 13       | 3.56          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 16       | 3.56          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 2        | 3.56          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 11       | 3.55          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 10       | 3.55          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 12       | 3.55          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 6        | 3.55          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 9        | 3.55          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 11       | 3.55          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 2        | 3.55          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 8        | 3.55          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 12       | 3.55          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 14       | 3.55          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 11       | 3.55          |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 15       | 3.55          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 9        | 3.54          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 12       | 3.54          |
| (1,725) | 1:55:A:VAL:H  | 1:87:A:SER:CB | 14       | 3.54          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 9        | 3.54          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 9        | 3.54          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 1        | 3.54          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 9        | 3.54          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 14       | 3.54          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 19       | 3.54          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 20       | 3.53          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 20       | 3.53          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 7        | 3.53          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 11       | 3.53          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 18       | 3.53          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 8        | 3.53          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 1        | 3.53          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 19       | 3.53          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 17       | 3.53          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 12       | 3.53          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 19       | 3.52          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 4        | 3.52          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 16       | 3.52          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 18       | 3.52          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 16       | 3.52          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 4        | 3.52          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 18       | 3.52          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 13       | 3.52          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 14       | 3.52          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 15       | 3.52          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 20       | 3.52          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 18       | 3.52          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 18       | 3.52          |
| (1,816) | 1:87:A:SER:CB | 1:96:A:LEU:H  | 15       | 3.51          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 6        | 3.51          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 8        | 3.51          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 7        | 3.51          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 2        | 3.51          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 6        | 3.51          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 11       | 3.51          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 11       | 3.51          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 15       | 3.51          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 10       | 3.51          |
| (1,679) | 1:47:A:SER:CB | 1:71:A:PHE:H  | 16       | 3.51          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 14       | 3.51          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 18       | 3.51          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 12       | 3.51          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 5        | 3.51          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 3        | 3.51          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 13       | 3.51          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 17       | 3.51          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 1        | 3.51          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 3        | 3.51          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 20       | 3.5           |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 3        | 3.5           |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 8        | 3.5           |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 13       | 3.5           |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 17       | 3.5           |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 8        | 3.5           |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 12       | 3.5           |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 15       | 3.5           |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 5        | 3.5           |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 13       | 3.5           |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 4        | 3.5           |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 14       | 3.5           |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 15       | 3.5           |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 5        | 3.49          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 5        | 3.49          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 1        | 3.49          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 19       | 3.49          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 4        | 3.49          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 19       | 3.49          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 3        | 3.49          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 6        | 3.49          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 14       | 3.49          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 5        | 3.49          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 9        | 3.49          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 2        | 3.49          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 16       | 3.49          |
| (1,434) | 1:16:A:SER:H  | 1:99:A:LEU:CB | 16       | 3.49          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 9        | 3.49          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 15       | 3.49          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 19       | 3.49          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 5        | 3.48          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 18       | 3.48          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 13       | 3.48          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 3        | 3.48          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 8        | 3.48          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 19       | 3.48          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 1        | 3.48          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 13       | 3.48          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 13       | 3.48          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 2        | 3.48          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 2        | 3.48          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 5        | 3.48          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 5        | 3.47          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 4        | 3.47          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 6        | 3.47          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 18       | 3.47          |
| (1,733) | 1:56:A:SER:CB | 1:74:A:SER:H  | 12       | 3.47          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 19       | 3.47          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 15       | 3.47          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 14       | 3.47          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 7        | 3.47          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 8        | 3.47          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 14       | 3.47          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 14       | 3.47          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 2        | 3.47          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 5        | 3.47          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 6        | 3.47          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 12       | 3.46          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 14       | 3.46          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 5        | 3.46          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 1        | 3.46          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 4        | 3.46          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 4        | 3.46          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 7        | 3.46          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 4        | 3.46          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 17       | 3.45          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 20       | 3.45          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 8        | 3.45          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 17       | 3.45          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 16       | 3.45          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 2        | 3.45          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 5        | 3.45          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 8        | 3.45          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 10       | 3.45          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 3        | 3.45          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 10       | 3.44          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 10       | 3.44          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 1        | 3.44          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 6        | 3.44          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 11       | 3.44          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 8        | 3.44          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 13       | 3.44          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 12       | 3.44          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 13       | 3.44          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 16       | 3.44          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 13       | 3.44          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 18       | 3.44          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 1        | 3.43          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 5        | 3.43          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 11       | 3.43          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 5        | 3.43          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 8        | 3.43          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 10       | 3.43          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 3        | 3.43          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 19       | 3.43          |
| (1,809) | 1:80:A:ALA:H  | 1:99:A:LEU:CB | 8        | 3.42          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 6        | 3.42          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 19       | 3.42          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 8        | 3.42          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 17       | 3.42          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 2        | 3.42          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 15       | 3.42          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 20       | 3.42          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 15       | 3.41          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 12       | 3.41          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 11       | 3.41          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 15       | 3.41          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 10       | 3.41          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 2        | 3.41          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 1        | 3.41          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 1        | 3.41          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 11       | 3.41          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 13       | 3.41          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 4        | 3.41          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 8        | 3.41          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 4        | 3.41          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 4        | 3.41          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 3        | 3.4           |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 20       | 3.4           |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 5        | 3.4           |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 6        | 3.4           |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 1        | 3.4           |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 4        | 3.39          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 15       | 3.39          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 20       | 3.39          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 12       | 3.39          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 3        | 3.39          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 13       | 3.39          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 11       | 3.39          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 10       | 3.39          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 16       | 3.39          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 15       | 3.38          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 8        | 3.38          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 19       | 3.38          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 1        | 3.38          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 17       | 3.38          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 3        | 3.38          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 11       | 3.38          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 1        | 3.38          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 12       | 3.38          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 1        | 3.37          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 12       | 3.37          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 16       | 3.37          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 17       | 3.37          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 20       | 3.37          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 7        | 3.37          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 18       | 3.37          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 11       | 3.37          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 11       | 3.37          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 10       | 3.37          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 20       | 3.37          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 15       | 3.37          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 18       | 3.37          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 4        | 3.37          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 9        | 3.37          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 19       | 3.37          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 6        | 3.37          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 3        | 3.37          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 6        | 3.37          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 19       | 3.36          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 12       | 3.36          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 2        | 3.36          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 18       | 3.36          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 19       | 3.36          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 12       | 3.36          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 17       | 3.36          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 5        | 3.36          |
| (1,406) | 1:12:A:VAL:H  | 1:37:A:CYS:CB | 16       | 3.36          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 10       | 3.35          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 15       | 3.35          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 17       | 3.35          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 1        | 3.35          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 15       | 3.35          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 4        | 3.35          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 7        | 3.35          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 1        | 3.35          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 20       | 3.35          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 20       | 3.35          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 2        | 3.35          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 2        | 3.34          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 10       | 3.34          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 16       | 3.34          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 7        | 3.34          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 7        | 3.34          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 10       | 3.34          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 9        | 3.34          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 13       | 3.34          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 2        | 3.34          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 2        | 3.34          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 20       | 3.34          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 13       | 3.34          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 14       | 3.34          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 15       | 3.34          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 2        | 3.34          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 3        | 3.34          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 13       | 3.34          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 1        | 3.33          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 16       | 3.33          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 13       | 3.33          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 9        | 3.33          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 19       | 3.33          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 13       | 3.33          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 12       | 3.33          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 4        | 3.33          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 6        | 3.33          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 12       | 3.33          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 12       | 3.33          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 11       | 3.32          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 14       | 3.32          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 14       | 3.32          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 8        | 3.32          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 3        | 3.32          |
| (1,574) | 1:31:A:ALA:H  | 1:87:A:SER:CB | 6        | 3.32          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 2        | 3.32          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 11       | 3.32          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 17       | 3.31          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 9        | 3.31          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 18       | 3.31          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 5        | 3.31          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 7        | 3.31          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 16       | 3.31          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 20       | 3.31          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 9        | 3.31          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 18       | 3.3           |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 11       | 3.3           |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 14       | 3.3           |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 14       | 3.3           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 14       | 3.3           |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 5        | 3.3           |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 3        | 3.3           |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 7        | 3.3           |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 7        | 3.3           |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 4        | 3.3           |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 2        | 3.3           |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 15       | 3.3           |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 15       | 3.3           |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 12       | 3.3           |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 18       | 3.3           |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 5        | 3.3           |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 14       | 3.3           |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 17       | 3.29          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 2        | 3.29          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 4        | 3.29          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 20       | 3.29          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 2        | 3.29          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 19       | 3.29          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 9        | 3.29          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 20       | 3.29          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 12       | 3.29          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 13       | 3.29          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 7        | 3.29          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 15       | 3.29          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 15       | 3.29          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 9        | 3.29          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 13       | 3.29          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 17       | 3.28          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 15       | 3.28          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 6        | 3.28          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 7        | 3.28          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 14       | 3.28          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 5        | 3.28          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 16       | 3.28          |
| (1,787) | 1:68:A:GLY:H  | 1:87:A:SER:CB | 16       | 3.27          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 14       | 3.27          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 13       | 3.27          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 18       | 3.27          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 11       | 3.27          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 16       | 3.27          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 13       | 3.27          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 19       | 3.27          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 20       | 3.27          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 14       | 3.27          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 8        | 3.27          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 3        | 3.27          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 7        | 3.27          |
| (1,449) | 1:19:A:GLY:H  | 1:87:A:SER:CB | 20       | 3.27          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 6        | 3.27          |
| (1,419) | 1:14:A:PHE:H  | 1:56:A:SER:CB | 13       | 3.27          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 3        | 3.27          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 9        | 3.27          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 15       | 3.27          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 19       | 3.26          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 12       | 3.26          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 5        | 3.26          |
| (1,650) | 1:42:A:GLY:H  | 1:87:A:SER:CB | 16       | 3.26          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 19       | 3.26          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 20       | 3.26          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 11       | 3.26          |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 12       | 3.26          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 1        | 3.26          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 10       | 3.25          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 7        | 3.25          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 2        | 3.25          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 4        | 3.25          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 2        | 3.25          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 18       | 3.25          |
| (1,618) | 1:37:A:CYS:CB | 1:80:A:ALA:H  | 3        | 3.25          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 14       | 3.25          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 9        | 3.25          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 9        | 3.25          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 12       | 3.25          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 9        | 3.25          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 10       | 3.25          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 1        | 3.25          |
| (1,774) | 1:63:A:LEU:H  | 1:99:A:LEU:CB | 1        | 3.24          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 20       | 3.24          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 6        | 3.24          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 9        | 3.24          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 4        | 3.24          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 19       | 3.24          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 17       | 3.24          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 19       | 3.24          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 13       | 3.24          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 10       | 3.24          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 2        | 3.24          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 12       | 3.24          |
| (1,608) | 1:37:A:CYS:CB | 1:62:A:PHE:H  | 9        | 3.24          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 20       | 3.24          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 19       | 3.24          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 11       | 3.24          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 15       | 3.23          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 13       | 3.23          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 13       | 3.23          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 8        | 3.23          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 1        | 3.23          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 10       | 3.23          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 16       | 3.23          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 3        | 3.23          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 16       | 3.23          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 19       | 3.23          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 11       | 3.23          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 1        | 3.22          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 15       | 3.22          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 2        | 3.22          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 13       | 3.22          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 13       | 3.22          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 1        | 3.22          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 13       | 3.22          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 10       | 3.22          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 14       | 3.22          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 12       | 3.22          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 8        | 3.22          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 10       | 3.22          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 18       | 3.22          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 8        | 3.22          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 13       | 3.22          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 12       | 3.22          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 4        | 3.21          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 9        | 3.21          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 6        | 3.21          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 14       | 3.21          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 4        | 3.21          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 7        | 3.21          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 4        | 3.21          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 18       | 3.21          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 10       | 3.21          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 11       | 3.21          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 5        | 3.21          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 10       | 3.21          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 6        | 3.21          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 20       | 3.21          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 20       | 3.21          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 20       | 3.21          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 16       | 3.21          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 17       | 3.21          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 16       | 3.21          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 4        | 3.2           |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 1        | 3.2           |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 1        | 3.2           |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 13       | 3.2           |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 10       | 3.2           |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 6        | 3.2           |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 13       | 3.2           |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 9        | 3.2           |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 5        | 3.2           |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 1        | 3.2           |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 16       | 3.19          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 8        | 3.19          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 18       | 3.19          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 12       | 3.19          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 20       | 3.19          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 15       | 3.19          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 19       | 3.19          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 14       | 3.19          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 1        | 3.19          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 18       | 3.19          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 8        | 3.19          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 4        | 3.19          |
| (1,404) | 1:11:A:LEU:H  | 1:87:A:SER:CB | 13       | 3.19          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 13       | 3.19          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 12       | 3.19          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 18       | 3.18          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 16       | 3.18          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 16       | 3.18          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 17       | 3.18          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 13       | 3.18          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 13       | 3.18          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 14       | 3.18          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 18       | 3.18          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 1        | 3.18          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 5        | 3.18          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 14       | 3.18          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 9        | 3.17          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 4        | 3.17          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 18       | 3.17          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 3        | 3.17          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 2        | 3.17          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 3        | 3.17          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 1        | 3.17          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 16       | 3.17          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 17       | 3.17          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 17       | 3.17          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 3        | 3.17          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 8        | 3.17          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 5        | 3.17          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 20       | 3.17          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 11       | 3.16          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 9        | 3.16          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 1        | 3.16          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 15       | 3.16          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 10       | 3.16          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 10       | 3.16          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 5        | 3.16          |
| (1,626) | 1:37:A:CYS:CB | 1:88:A:LEU:H  | 20       | 3.16          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 14       | 3.16          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 15       | 3.16          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 4        | 3.16          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 10       | 3.16          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 11       | 3.16          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 14       | 3.16          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 15       | 3.16          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 16       | 3.16          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 14       | 3.16          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 18       | 3.16          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 9        | 3.16          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 2        | 3.15          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 19       | 3.15          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 18       | 3.15          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 14       | 3.15          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 16       | 3.15          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 20       | 3.15          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 20       | 3.15          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 16       | 3.15          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 4        | 3.15          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 2        | 3.15          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 9        | 3.15          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 16       | 3.15          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 7        | 3.15          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 5        | 3.15          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 12       | 3.15          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 17       | 3.15          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 6        | 3.15          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 13       | 3.15          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 1        | 3.15          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 3        | 3.14          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 1        | 3.14          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 16       | 3.14          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 15       | 3.14          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 14       | 3.14          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 16       | 3.14          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 1        | 3.14          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 15       | 3.14          |
| (1,393) | 1:10:A:ALA:H  | 1:37:A:CYS:CB | 4        | 3.14          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 7        | 3.13          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 20       | 3.13          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 18       | 3.13          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 16       | 3.13          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 19       | 3.13          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 13       | 3.13          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 18       | 3.13          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 5        | 3.13          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 13       | 3.13          |
| (1,498) | 1:20:A:TYR:CB | 1:76:A:LYS:H  | 10       | 3.13          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 13       | 3.13          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 13       | 3.13          |
| (1,378) | 1:8:A:TYR:H   | 1:20:A:TYR:CB | 16       | 3.13          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 19       | 3.13          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 10       | 3.12          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 20       | 3.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 3        | 3.12          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 12       | 3.12          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 1        | 3.12          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 6        | 3.12          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 20       | 3.12          |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 9        | 3.12          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 5        | 3.12          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 16       | 3.12          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 20       | 3.12          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 15       | 3.12          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 11       | 3.12          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 17       | 3.11          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 19       | 3.11          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 10       | 3.11          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 7        | 3.11          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 16       | 3.11          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 14       | 3.11          |
| (1,653) | 1:43:A:ALA:H  | 1:87:A:SER:CB | 16       | 3.11          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 19       | 3.11          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 6        | 3.11          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 11       | 3.11          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 9        | 3.11          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 12       | 3.1           |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 16       | 3.1           |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 11       | 3.1           |
| (1,655) | 1:44:A:TYR:H  | 1:56:A:SER:CB | 18       | 3.1           |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 17       | 3.1           |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 10       | 3.1           |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 11       | 3.1           |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 13       | 3.1           |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 14       | 3.1           |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 8        | 3.1           |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 4        | 3.1           |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 5        | 3.1           |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 12       | 3.09          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 14       | 3.09          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 7        | 3.09          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 13       | 3.09          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 12       | 3.09          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 4        | 3.09          |
| (1,615) | 1:37:A:CYS:CB | 1:69:A:VAL:H  | 2        | 3.09          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 10       | 3.09          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 7        | 3.09          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 17       | 3.09          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 9        | 3.09          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 17       | 3.09          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 13       | 3.09          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 16       | 3.08          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 2        | 3.08          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 11       | 3.08          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 18       | 3.08          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 19       | 3.08          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 13       | 3.08          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 11       | 3.08          |
| (1,641) | 1:40:A:GLY:H  | 1:47:A:SER:CB | 20       | 3.08          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 11       | 3.08          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 15       | 3.08          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 16       | 3.08          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 11       | 3.08          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 17       | 3.08          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 14       | 3.08          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 11       | 3.08          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 16       | 3.07          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 2        | 3.07          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 8        | 3.07          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 5        | 3.07          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 6        | 3.07          |
| (1,493) | 1:20:A:TYR:CB | 1:72:A:LYS:H  | 9        | 3.07          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 12       | 3.07          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 5        | 3.06          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 10       | 3.06          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 20       | 3.06          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 6        | 3.06          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 11       | 3.06          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 15       | 3.06          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 19       | 3.06          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 9        | 3.06          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 5        | 3.06          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 20       | 3.06          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 2        | 3.06          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 15       | 3.06          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 5        | 3.06          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 12       | 3.06          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 18       | 3.06          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 19       | 3.06          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 12       | 3.06          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 12       | 3.05          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 15       | 3.05          |
| (1,773) | 1:63:A:LEU:H  | 1:87:A:SER:CB | 17       | 3.05          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 17       | 3.05          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 6        | 3.05          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 14       | 3.05          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 8        | 3.05          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 20       | 3.05          |
| (1,723) | 1:54:A:LYS:H  | 1:87:A:SER:CB | 5        | 3.05          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 13       | 3.05          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 14       | 3.05          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 4        | 3.05          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 18       | 3.05          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 7        | 3.05          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 2        | 3.05          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 13       | 3.05          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 4        | 3.05          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 8        | 3.05          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 18       | 3.05          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 4        | 3.05          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 3        | 3.04          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 10       | 3.04          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 3        | 3.04          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 14       | 3.04          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 5        | 3.04          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 10       | 3.04          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 6        | 3.04          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 2        | 3.04          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 9        | 3.04          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 18       | 3.04          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 13       | 3.03          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 19       | 3.03          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 5        | 3.03          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 18       | 3.03          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 2        | 3.03          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 18       | 3.03          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 2        | 3.03          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 3        | 3.03          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 3        | 3.03          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 19       | 3.03          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 5        | 3.03          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 1        | 3.03          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 16       | 3.02          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 19       | 3.02          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 8        | 3.02          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 7        | 3.02          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 2        | 3.02          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 15       | 3.02          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 18       | 3.02          |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 12       | 3.02          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 9        | 3.02          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 12       | 3.02          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 17       | 3.02          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 5        | 3.01          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 12       | 3.01          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 15       | 3.01          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 6        | 3.01          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 4        | 3.01          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 10       | 3.01          |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 5        | 3.01          |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 6        | 3.01          |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 10       | 3.01          |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 11       | 3.01          |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 13       | 3.01          |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 14       | 3.01          |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 17       | 3.01          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 20       | 3.01          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 10       | 3.01          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 12       | 3.01          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 13       | 3.01          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 11       | 3.01          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 2        | 3.01          |
| (1,445) | 1:19:A:GLY:H  | 1:37:A:CYS:CB | 2        | 3.01          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 16       | 3.01          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 14       | 3.01          |
| (1,341) | 1:2:A:ASP:H   | 1:74:A:SER:CB | 5        | 3.01          |
| (1,779) | 1:65:A:THR:H  | 1:99:A:LEU:CB | 11       | 3.0           |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 8        | 3.0           |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 11       | 3.0           |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 1        | 3.0           |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 2        | 3.0           |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 3        | 3.0           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 4        | 3.0           |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 7        | 3.0           |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 8        | 3.0           |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 9        | 3.0           |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 15       | 3.0           |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 16       | 3.0           |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 18       | 3.0           |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 20       | 3.0           |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 6        | 3.0           |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 15       | 3.0           |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 8        | 3.0           |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 7        | 3.0           |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 15       | 3.0           |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 18       | 3.0           |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 16       | 2.99          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 7        | 2.99          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 3        | 2.99          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 20       | 2.99          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 16       | 2.99          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 9        | 2.99          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 6        | 2.99          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 7        | 2.99          |
| (1,555) | 1:26:A:VAL:H  | 1:99:A:LEU:CB | 14       | 2.99          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 6        | 2.99          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 14       | 2.98          |
| (1,647) | 1:41:A:TYR:H  | 1:87:A:SER:CB | 19       | 2.98          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 7        | 2.98          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 9        | 2.98          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 14       | 2.98          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 8        | 2.98          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 5        | 2.98          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 5        | 2.98          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 19       | 2.98          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 17       | 2.98          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 13       | 2.98          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 18       | 2.98          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 17       | 2.97          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 12       | 2.97          |
| (1,727) | 1:56:A:SER:CB | 1:63:A:LEU:H  | 13       | 2.97          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 15       | 2.97          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 17       | 2.97          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 4        | 2.97          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 16       | 2.97          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 12       | 2.97          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 2        | 2.97          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 10       | 2.97          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 2        | 2.96          |
| (1,707) | 1:49:A:ASP:H  | 1:56:A:SER:CB | 3        | 2.96          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 20       | 2.96          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 16       | 2.96          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 8        | 2.96          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 8        | 2.96          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 12       | 2.96          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 4        | 2.96          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 16       | 2.96          |
| (1,458) | 1:20:A:TYR:H  | 1:37:A:CYS:CB | 2        | 2.96          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 9        | 2.96          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 11       | 2.96          |
| (1,347) | 1:3:A:LEU:H   | 1:74:A:SER:CB | 5        | 2.96          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 4        | 2.95          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 13       | 2.95          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 14       | 2.95          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 14       | 2.95          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 15       | 2.95          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 7        | 2.95          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 12       | 2.95          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 8        | 2.95          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 13       | 2.95          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 1        | 2.95          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 20       | 2.95          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 3        | 2.95          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 7        | 2.94          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 10       | 2.94          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 13       | 2.94          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 15       | 2.94          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 17       | 2.94          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 6        | 2.94          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 17       | 2.94          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 11       | 2.94          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 2        | 2.94          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 11       | 2.94          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 10       | 2.94          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 13       | 2.94          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 11       | 2.94          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 4        | 2.94          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 2        | 2.94          |
| (1,527) | 1:21:A:LYS:H  | 1:87:A:SER:CB | 5        | 2.94          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 17       | 2.94          |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 4        | 2.94          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 3        | 2.94          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 7        | 2.94          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 3        | 2.93          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 20       | 2.93          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 5        | 2.93          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 10       | 2.93          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 14       | 2.93          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 7        | 2.93          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 1        | 2.93          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 15       | 2.93          |
| (1,629) | 1:37:A:CYS:CB | 1:91:A:ILE:H  | 20       | 2.93          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 12       | 2.93          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 18       | 2.93          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 6        | 2.93          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 4        | 2.93          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 11       | 2.93          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 4        | 2.93          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 12       | 2.93          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 5        | 2.93          |
| (1,489) | 1:20:A:TYR:CB | 1:68:A:GLY:H  | 2        | 2.93          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 4        | 2.93          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 1        | 2.93          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 8        | 2.93          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 3        | 2.93          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 6        | 2.93          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 6        | 2.92          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 9        | 2.92          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 12       | 2.92          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 10       | 2.92          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 11       | 2.92          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 4        | 2.92          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 14       | 2.92          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 20       | 2.92          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 12       | 2.92          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 15       | 2.92          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 4        | 2.92          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 18       | 2.92          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 5        | 2.92          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 9        | 2.92          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 12       | 2.92          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 1        | 2.92          |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 9        | 2.92          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 10       | 2.92          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 4        | 2.92          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 1        | 2.92          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 5        | 2.92          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 3        | 2.91          |
| (1,688) | 1:47:A:SER:CB | 1:84:A:ALA:H  | 9        | 2.91          |
| (1,686) | 1:47:A:SER:CB | 1:82:A:LEU:H  | 5        | 2.91          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 1        | 2.91          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 10       | 2.91          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 13       | 2.91          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 11       | 2.91          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 19       | 2.91          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 7        | 2.91          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 13       | 2.91          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 1        | 2.9           |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 12       | 2.9           |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 14       | 2.9           |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 9        | 2.9           |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 5        | 2.9           |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 9        | 2.9           |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 8        | 2.9           |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 1        | 2.9           |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 4        | 2.9           |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 16       | 2.9           |
| (1,630) | 1:37:A:CYS:CB | 1:92:A:LEU:H  | 19       | 2.9           |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 17       | 2.9           |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 18       | 2.9           |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 15       | 2.9           |
| (1,363) | 1:5:A:GLY:H   | 1:99:A:LEU:CB | 16       | 2.9           |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 2        | 2.89          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 13       | 2.89          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 19       | 2.89          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 1        | 2.89          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 17       | 2.89          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 12       | 2.89          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 15       | 2.89          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 14       | 2.89          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 1        | 2.89          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 15       | 2.89          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 13       | 2.88          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 5        | 2.88          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 19       | 2.88          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 8        | 2.88          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 20       | 2.88          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 8        | 2.88          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 12       | 2.88          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 16       | 2.88          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 11       | 2.88          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 13       | 2.88          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 3        | 2.88          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 6        | 2.88          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 13       | 2.88          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 3        | 2.88          |
| (1,470) | 1:20:A:TYR:CB | 1:50:A:LYS:H  | 19       | 2.88          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 4        | 2.88          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 1        | 2.87          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 2        | 2.87          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 1        | 2.87          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 15       | 2.87          |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 17       | 2.87          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 6        | 2.87          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 12       | 2.87          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 16       | 2.87          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 7        | 2.87          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 19       | 2.87          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 3        | 2.87          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 19       | 2.87          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 7        | 2.87          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 19       | 2.87          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 19       | 2.87          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 1        | 2.87          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 9        | 2.87          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 4        | 2.86          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 18       | 2.86          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 18       | 2.86          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 5        | 2.86          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 1        | 2.86          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 1        | 2.86          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 1        | 2.86          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 17       | 2.86          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 20       | 2.86          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 3        | 2.86          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 3        | 2.86          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 1        | 2.86          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 2        | 2.86          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 14       | 2.85          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 2        | 2.85          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 2        | 2.85          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 6        | 2.85          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 1        | 2.85          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 6        | 2.85          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 9        | 2.85          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 18       | 2.85          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 8        | 2.85          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 17       | 2.85          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 5        | 2.85          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 11       | 2.85          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 10       | 2.85          |
| (1,571) | 1:31:A:ALA:H  | 1:47:A:SER:CB | 19       | 2.85          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 12       | 2.85          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 3        | 2.85          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 19       | 2.85          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 2        | 2.85          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 20       | 2.85          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 13       | 2.84          |
| (1,588) | 1:35:A:VAL:H  | 1:99:A:LEU:CB | 12       | 2.84          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 2        | 2.84          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 20       | 2.84          |
| (1,476) | 1:20:A:TYR:CB | 1:56:A:SER:H  | 1        | 2.84          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 11       | 2.84          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 11       | 2.83          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 20       | 2.83          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 19       | 2.83          |
| (1,706) | 1:48:A:ASN:H  | 1:99:A:LEU:CB | 2        | 2.83          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 1        | 2.83          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 2        | 2.83          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 17       | 2.83          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 13       | 2.82          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 15       | 2.82          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 8        | 2.82          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 13       | 2.82          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 9        | 2.82          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 11       | 2.82          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 3        | 2.82          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 3        | 2.82          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 3        | 2.81          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 20       | 2.81          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 17       | 2.81          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 18       | 2.81          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 6        | 2.81          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 10       | 2.81          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 5        | 2.81          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 10       | 2.81          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 3        | 2.81          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 4        | 2.81          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 16       | 2.81          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 14       | 2.81          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 15       | 2.81          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 17       | 2.81          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 20       | 2.81          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 16       | 2.8           |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 20       | 2.8           |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 4        | 2.8           |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 9        | 2.8           |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 9        | 2.8           |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 3        | 2.8           |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 1        | 2.8           |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 1        | 2.8           |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 3        | 2.8           |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 8        | 2.8           |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 8        | 2.8           |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 8        | 2.8           |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 16       | 2.8           |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 14       | 2.8           |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 7        | 2.8           |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 7        | 2.8           |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 14       | 2.8           |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 15       | 2.79          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 18       | 2.79          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 2        | 2.79          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 7        | 2.79          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 16       | 2.79          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 8        | 2.79          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 2        | 2.79          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 19       | 2.79          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 1        | 2.79          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 1        | 2.79          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 7        | 2.79          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 15       | 2.79          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 4        | 2.79          |
| (1,400) | 1:11:A:LEU:H  | 1:37:A:CYS:CB | 6        | 2.79          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 8        | 2.78          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 19       | 2.78          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 5        | 2.78          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 18       | 2.78          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 8        | 2.78          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 8        | 2.78          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 4        | 2.78          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 20       | 2.78          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 6        | 2.78          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 18       | 2.78          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 14       | 2.78          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 7        | 2.77          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 1        | 2.77          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 12       | 2.77          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 9        | 2.77          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 17       | 2.77          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 8        | 2.77          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 4        | 2.77          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 9        | 2.77          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 12       | 2.77          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 8        | 2.77          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 5        | 2.77          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 20       | 2.77          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 14       | 2.77          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 3        | 2.77          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 19       | 2.77          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 13       | 2.77          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 8        | 2.77          |
| (1,384) | 1:8:A:TYR:H   | 1:99:A:LEU:CB | 16       | 2.77          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 7        | 2.76          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 1        | 2.76          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 1        | 2.76          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 19       | 2.76          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 9        | 2.76          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 9        | 2.76          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 12       | 2.76          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 12       | 2.76          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 3        | 2.76          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 4        | 2.76          |
| (1,603) | 1:37:A:CYS:CB | 1:57:A:LEU:H  | 4        | 2.76          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 9        | 2.76          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 2        | 2.76          |
| (1,479) | 1:20:A:TYR:CB | 1:58:A:PHE:H  | 19       | 2.76          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 7        | 2.76          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 20       | 2.76          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 16       | 2.75          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 20       | 2.75          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 12       | 2.75          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 15       | 2.75          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 13       | 2.75          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 2        | 2.75          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 8        | 2.75          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 20       | 2.75          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 19       | 2.75          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 11       | 2.75          |
| (1,771) | 1:62:A:PHE:H  | 1:99:A:LEU:CB | 11       | 2.74          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 10       | 2.74          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 4        | 2.74          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 13       | 2.74          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 14       | 2.74          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 11       | 2.74          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 5        | 2.74          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 8        | 2.74          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 18       | 2.74          |
| (1,483) | 1:20:A:TYR:CB | 1:62:A:PHE:H  | 9        | 2.74          |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 15       | 2.74          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 15       | 2.74          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 6        | 2.74          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 4        | 2.73          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 6        | 2.73          |
| (1,520) | 1:20:A:TYR:CB | 1:98:A:LEU:H  | 15       | 2.73          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 6        | 2.73          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 17       | 2.73          |
| (1,356) | 1:4:A:ILE:H   | 1:99:A:LEU:CB | 16       | 2.73          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 18       | 2.72          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 13       | 2.72          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 18       | 2.72          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 13       | 2.72          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 3        | 2.72          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 10       | 2.72          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 17       | 2.72          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 6        | 2.72          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 1        | 2.72          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 4        | 2.72          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 19       | 2.72          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 1        | 2.72          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 9        | 2.72          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 14       | 2.72          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 11       | 2.72          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 17       | 2.72          |
| (1,462) | 1:20:A:TYR:CB | 1:42:A:GLY:H  | 4        | 2.72          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 3        | 2.72          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 5        | 2.72          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 10       | 2.72          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 13       | 2.72          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 11       | 2.71          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 3        | 2.71          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 2        | 2.71          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 9        | 2.71          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 12       | 2.71          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 15       | 2.71          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 3        | 2.71          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 7        | 2.71          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 19       | 2.71          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 9        | 2.71          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 18       | 2.71          |
| (1,487) | 1:20:A:TYR:CB | 1:66:A:ILE:H  | 14       | 2.71          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 5        | 2.7           |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 6        | 2.7           |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 7        | 2.7           |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 20       | 2.7           |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 19       | 2.7           |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 18       | 2.7           |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 20       | 2.7           |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 8        | 2.7           |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 13       | 2.7           |
| (1,490) | 1:20:A:TYR:CB | 1:69:A:VAL:H  | 2        | 2.7           |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 1        | 2.69          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 6        | 2.69          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 6        | 2.69          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 8        | 2.69          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 6        | 2.69          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 2        | 2.69          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 14       | 2.69          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 18       | 2.69          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 3        | 2.69          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 7        | 2.69          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 4        | 2.69          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 3        | 2.69          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 3        | 2.69          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 17       | 2.69          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 6        | 2.69          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 10       | 2.69          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 10       | 2.68          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 7        | 2.68          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 10       | 2.68          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 17       | 2.68          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 18       | 2.68          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 1        | 2.68          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 15       | 2.68          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 11       | 2.68          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 4        | 2.68          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 1        | 2.68          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 13       | 2.68          |
| (1,431) | 1:16:A:SER:H  | 1:56:A:SER:CB | 16       | 2.68          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 20       | 2.67          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 1        | 2.67          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 6        | 2.67          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 5        | 2.67          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 7        | 2.67          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 11       | 2.67          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 7        | 2.67          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 10       | 2.67          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 14       | 2.67          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 19       | 2.67          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 6        | 2.67          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 3        | 2.67          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 10       | 2.67          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 6        | 2.67          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 9        | 2.67          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 11       | 2.67          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 8        | 2.66          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 4        | 2.66          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 3        | 2.66          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 11       | 2.66          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 3        | 2.66          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 20       | 2.66          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 2        | 2.66          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 4        | 2.66          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 17       | 2.66          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 1        | 2.66          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 8        | 2.66          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 7        | 2.66          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 17       | 2.66          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 7        | 2.65          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 8        | 2.65          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 8        | 2.65          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 12       | 2.65          |
| (1,722) | 1:54:A:LYS:H  | 1:74:A:SER:CB | 5        | 2.65          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 15       | 2.65          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 14       | 2.65          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 18       | 2.65          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 11       | 2.65          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 1        | 2.65          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 14       | 2.65          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 9        | 2.65          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 17       | 2.64          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 8        | 2.64          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 9        | 2.64          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 2        | 2.64          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 10       | 2.64          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 9        | 2.64          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 6        | 2.64          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 16       | 2.64          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 5        | 2.64          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 7        | 2.64          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 7        | 2.64          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 6        | 2.64          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 11       | 2.64          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 17       | 2.64          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 3        | 2.64          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 16       | 2.64          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 14       | 2.64          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 13       | 2.64          |
| (1,532) | 1:22:A:ARG:H  | 1:99:A:LEU:CB | 10       | 2.64          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 18       | 2.64          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 1        | 2.64          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 6        | 2.64          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 17       | 2.63          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 19       | 2.63          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 3        | 2.63          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 12       | 2.63          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 17       | 2.63          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 18       | 2.63          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 20       | 2.63          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 19       | 2.63          |
| (1,473) | 1:20:A:TYR:CB | 1:53:A:VAL:H  | 5        | 2.63          |
| (1,428) | 1:15:A:GLY:H  | 1:99:A:LEU:CB | 20       | 2.63          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 14       | 2.62          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 7        | 2.62          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 17       | 2.62          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 17       | 2.62          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 16       | 2.62          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 8        | 2.62          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 14       | 2.62          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 3        | 2.62          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 3        | 2.62          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 5        | 2.62          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 19       | 2.62          |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 20       | 2.61          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 14       | 2.61          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 18       | 2.61          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 5        | 2.61          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 9        | 2.61          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 1        | 2.61          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 13       | 2.61          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 2        | 2.61          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 10       | 2.61          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 9        | 2.61          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 14       | 2.61          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 13       | 2.61          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 8        | 2.61          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 8        | 2.61          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 14       | 2.61          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 15       | 2.6           |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 12       | 2.6           |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 1        | 2.6           |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 9        | 2.6           |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 17       | 2.6           |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 7        | 2.6           |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 6        | 2.6           |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 20       | 2.6           |
| (1,569) | 1:30:A:ILE:H  | 1:87:A:SER:CB | 6        | 2.6           |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 17       | 2.6           |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 10       | 2.6           |
| (1,464) | 1:20:A:TYR:CB | 1:44:A:TYR:H  | 19       | 2.6           |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 11       | 2.6           |
| (1,820) | 1:87:A:SER:H  | 1:99:A:LEU:CB | 10       | 2.59          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 20       | 2.59          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 9        | 2.59          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 11       | 2.59          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 16       | 2.59          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 14       | 2.59          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 5        | 2.59          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 9        | 2.59          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 3        | 2.59          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 10       | 2.59          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 19       | 2.59          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 20       | 2.59          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 2        | 2.58          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 4        | 2.58          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 6        | 2.58          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 5        | 2.58          |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 14       | 2.58          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 15       | 2.58          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 5        | 2.58          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 16       | 2.58          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 18       | 2.58          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 7        | 2.58          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 12       | 2.58          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 4        | 2.58          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 18       | 2.58          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 7        | 2.58          |
| (1,517) | 1:20:A:TYR:CB | 1:95:A:VAL:H  | 19       | 2.58          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 4        | 2.58          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 19       | 2.58          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 20       | 2.58          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 1        | 2.57          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 4        | 2.57          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 18       | 2.57          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 4        | 2.57          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 17       | 2.57          |
| (1,616) | 1:37:A:CYS:CB | 1:70:A:ARG:H  | 7        | 2.57          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 10       | 2.57          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 5        | 2.57          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 18       | 2.57          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 13       | 2.57          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 2        | 2.57          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 12       | 2.56          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 19       | 2.56          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 20       | 2.56          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 2        | 2.56          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 6        | 2.56          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 6        | 2.56          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 16       | 2.56          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 8        | 2.56          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 11       | 2.56          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 8        | 2.56          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 19       | 2.56          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 13       | 2.55          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 19       | 2.55          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 11       | 2.55          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 3        | 2.55          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 7        | 2.55          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 9        | 2.55          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 11       | 2.55          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 15       | 2.55          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 20       | 2.55          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 12       | 2.55          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 11       | 2.55          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 18       | 2.55          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 9        | 2.55          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 17       | 2.55          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 19       | 2.55          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 8        | 2.54          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 18       | 2.54          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 19       | 2.54          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 12       | 2.54          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 15       | 2.54          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 4        | 2.54          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 14       | 2.54          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 12       | 2.54          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 6        | 2.54          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 13       | 2.54          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 8        | 2.54          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 12       | 2.54          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 5        | 2.54          |
| (1,801) | 1:74:A:SER:CB | 1:94:A:LEU:H  | 3        | 2.53          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 15       | 2.53          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 16       | 2.53          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 2        | 2.53          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 8        | 2.53          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 2        | 2.53          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 11       | 2.53          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 7        | 2.53          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 1        | 2.53          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 10       | 2.53          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 2        | 2.53          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 16       | 2.53          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 18       | 2.53          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 6        | 2.53          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 10       | 2.53          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 7        | 2.53          |
| (1,482) | 1:20:A:TYR:CB | 1:61:A:PHE:H  | 2        | 2.53          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 14       | 2.53          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 5        | 2.53          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 6        | 2.52          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 5        | 2.52          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 12       | 2.52          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 19       | 2.52          |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 10       | 2.52          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 18       | 2.52          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 19       | 2.52          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 12       | 2.52          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 7        | 2.52          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 6        | 2.52          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 20       | 2.52          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 16       | 2.52          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 16       | 2.51          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 3        | 2.51          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 15       | 2.51          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 4        | 2.51          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 18       | 2.51          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 18       | 2.51          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 4        | 2.51          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 13       | 2.51          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 6        | 2.5           |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 20       | 2.5           |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 16       | 2.5           |
| (1,663) | 1:47:A:SER:CB | 1:53:A:VAL:H  | 17       | 2.5           |
| (1,651) | 1:42:A:GLY:H  | 1:99:A:LEU:CB | 2        | 2.5           |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 19       | 2.5           |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 2        | 2.5           |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 5        | 2.5           |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 14       | 2.5           |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 10       | 2.5           |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 12       | 2.5           |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 16       | 2.5           |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 11       | 2.5           |
| (1,471) | 1:20:A:TYR:CB | 1:51:A:ARG:H  | 19       | 2.5           |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 11       | 2.5           |
| (1,371) | 1:7:A:GLY:H   | 1:20:A:TYR:CB | 16       | 2.5           |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 5        | 2.49          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 13       | 2.49          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 12       | 2.49          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 11       | 2.49          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 13       | 2.49          |
| (1,598) | 1:37:A:CYS:CB | 1:50:A:LYS:H  | 19       | 2.49          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 10       | 2.49          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 19       | 2.49          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 2        | 2.49          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 13       | 2.49          |
| (1,542) | 1:24:A:GLY:H  | 1:87:A:SER:CB | 14       | 2.49          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 18       | 2.49          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 2        | 2.49          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 20       | 2.48          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 4        | 2.48          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 11       | 2.48          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 11       | 2.48          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 15       | 2.48          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 1        | 2.48          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 1        | 2.48          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 17       | 2.48          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 18       | 2.47          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 6        | 2.47          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 9        | 2.47          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 9        | 2.47          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 4        | 2.47          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 2        | 2.47          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 5        | 2.47          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 7        | 2.47          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 16       | 2.47          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 15       | 2.47          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 18       | 2.47          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 20       | 2.47          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 1        | 2.47          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 20       | 2.46          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 16       | 2.46          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 18       | 2.46          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 3        | 2.46          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 2        | 2.46          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 6        | 2.46          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 18       | 2.46          |
| (1,573) | 1:31:A:ALA:H  | 1:74:A:SER:CB | 16       | 2.46          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 13       | 2.46          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 19       | 2.46          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 4        | 2.46          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 12       | 2.45          |
| (1,582) | 1:33:A:LEU:H  | 1:87:A:SER:CB | 6        | 2.45          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 6        | 2.45          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 13       | 2.45          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 11       | 2.45          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 3        | 2.45          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 8        | 2.45          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 3        | 2.45          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 18       | 2.45          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 17       | 2.45          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 14       | 2.44          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 12       | 2.44          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 15       | 2.44          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 4        | 2.44          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 3        | 2.44          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 8        | 2.44          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 18       | 2.44          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 10       | 2.44          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 8        | 2.44          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 2        | 2.44          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 7        | 2.44          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 19       | 2.44          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 10       | 2.44          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 7        | 2.43          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 8        | 2.43          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 13       | 2.43          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 19       | 2.43          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 5        | 2.43          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 11       | 2.43          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 8        | 2.43          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 17       | 2.43          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 7        | 2.43          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 8        | 2.42          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 7        | 2.42          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 15       | 2.42          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 19       | 2.42          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 8        | 2.42          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 12       | 2.42          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 4        | 2.42          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 13       | 2.42          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 11       | 2.42          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 3        | 2.42          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 4        | 2.42          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 15       | 2.42          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 5        | 2.42          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 6        | 2.42          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 5        | 2.41          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 8        | 2.41          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 15       | 2.41          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 9        | 2.41          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 14       | 2.41          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 19       | 2.41          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 7        | 2.41          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 4        | 2.41          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 8        | 2.41          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 18       | 2.41          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 4        | 2.41          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 1        | 2.41          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 4        | 2.41          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 17       | 2.41          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 19       | 2.41          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 14       | 2.41          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 1        | 2.41          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 11       | 2.41          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 11       | 2.4           |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 12       | 2.4           |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 19       | 2.4           |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 14       | 2.4           |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 20       | 2.4           |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 9        | 2.4           |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 1        | 2.4           |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 20       | 2.4           |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 10       | 2.4           |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 12       | 2.4           |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 7        | 2.4           |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 13       | 2.4           |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 2        | 2.4           |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 15       | 2.4           |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 2        | 2.39          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 5        | 2.39          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 4        | 2.39          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 7        | 2.39          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 8        | 2.39          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 8        | 2.39          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 20       | 2.39          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 6        | 2.39          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 10       | 2.39          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 12       | 2.38          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 14       | 2.38          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 10       | 2.38          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 6        | 2.38          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 7        | 2.38          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 14       | 2.38          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 10       | 2.38          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 13       | 2.38          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 3        | 2.38          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 19       | 2.38          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 16       | 2.38          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 4        | 2.38          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 17       | 2.38          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 8        | 2.37          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 17       | 2.37          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 4        | 2.37          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 11       | 2.37          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 15       | 2.37          |
| (1,724) | 1:55:A:VAL:H  | 1:74:A:SER:CB | 2        | 2.37          |
| (1,719) | 1:53:A:VAL:H  | 1:74:A:SER:CB | 5        | 2.37          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 18       | 2.37          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 19       | 2.37          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 2        | 2.37          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 9        | 2.37          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 15       | 2.37          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 7        | 2.37          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 13       | 2.37          |
| (1,502) | 1:20:A:TYR:CB | 1:81:A:GLY:H  | 11       | 2.37          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 11       | 2.37          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 11       | 2.37          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 13       | 2.37          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 17       | 2.37          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 10       | 2.36          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 10       | 2.36          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 9        | 2.36          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 15       | 2.36          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 12       | 2.36          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 4        | 2.36          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 13       | 2.36          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 9        | 2.36          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 10       | 2.36          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 4        | 2.36          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 10       | 2.36          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 19       | 2.36          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 5        | 2.36          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 18       | 2.36          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 2        | 2.36          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 15       | 2.36          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 14       | 2.36          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 2        | 2.36          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 18       | 2.36          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 8        | 2.35          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 1        | 2.35          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 4        | 2.35          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 5        | 2.35          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 17       | 2.35          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 14       | 2.35          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 4        | 2.35          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 19       | 2.35          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 13       | 2.34          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 11       | 2.34          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 19       | 2.34          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 9        | 2.34          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 19       | 2.34          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 1        | 2.34          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 15       | 2.34          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 8        | 2.34          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 10       | 2.34          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 1        | 2.34          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 4        | 2.34          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 5        | 2.34          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 9        | 2.34          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 20       | 2.34          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 9        | 2.34          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 17       | 2.34          |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 14       | 2.34          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 19       | 2.33          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 4        | 2.33          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 19       | 2.33          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 18       | 2.33          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 7        | 2.33          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 11       | 2.33          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 1        | 2.33          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 8        | 2.33          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 18       | 2.32          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 15       | 2.32          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 10       | 2.32          |
| (1,643) | 1:40:A:GLY:H  | 1:87:A:SER:CB | 16       | 2.32          |
| (1,632) | 1:37:A:CYS:CB | 1:94:A:LEU:H  | 20       | 2.32          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 3        | 2.32          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 4        | 2.32          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 19       | 2.32          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 18       | 2.32          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 10       | 2.31          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 20       | 2.31          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 2        | 2.31          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 13       | 2.31          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 18       | 2.31          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 15       | 2.31          |
| (1,596) | 1:37:A:CYS:CB | 1:48:A:ASN:H  | 20       | 2.31          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 14       | 2.31          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 7        | 2.31          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 15       | 2.31          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 18       | 2.31          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 11       | 2.31          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 5        | 2.31          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 10       | 2.31          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 2        | 2.31          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 5        | 2.31          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 2        | 2.31          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 3        | 2.3           |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 16       | 2.3           |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 18       | 2.3           |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 4        | 2.3           |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 16       | 2.3           |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 16       | 2.3           |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 2        | 2.3           |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 9        | 2.3           |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 5        | 2.3           |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 10       | 2.29          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 10       | 2.29          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 14       | 2.29          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 8        | 2.29          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 15       | 2.29          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 16       | 2.29          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 17       | 2.29          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 19       | 2.29          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 13       | 2.29          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 14       | 2.28          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 13       | 2.28          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 16       | 2.28          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 14       | 2.28          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 2        | 2.28          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 8        | 2.28          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 4        | 2.28          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 16       | 2.28          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 11       | 2.28          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 6        | 2.28          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 17       | 2.28          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 3        | 2.28          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 3        | 2.28          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 16       | 2.28          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 9        | 2.27          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 15       | 2.27          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 19       | 2.27          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 18       | 2.27          |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 20       | 2.27          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 9        | 2.27          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 17       | 2.27          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 7        | 2.27          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 17       | 2.27          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 9        | 2.27          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 11       | 2.27          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 8        | 2.26          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 14       | 2.26          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 8        | 2.26          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 15       | 2.26          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 3        | 2.26          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 14       | 2.26          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 2        | 2.26          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 6        | 2.26          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 3        | 2.26          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 8        | 2.26          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 1        | 2.26          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 14       | 2.26          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 6        | 2.26          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 20       | 2.26          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 10       | 2.26          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 6        | 2.26          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 7        | 2.26          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 13       | 2.26          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 6        | 2.25          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 7        | 2.25          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 5        | 2.25          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 19       | 2.25          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 5        | 2.25          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 7        | 2.25          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 5        | 2.25          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 19       | 2.25          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 13       | 2.25          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 17       | 2.25          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 17       | 2.25          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 15       | 2.25          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 7        | 2.24          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 12       | 2.24          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 5        | 2.24          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 15       | 2.24          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 1        | 2.24          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 4        | 2.24          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 13       | 2.24          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 5        | 2.24          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 11       | 2.24          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 3        | 2.24          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 20       | 2.24          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 19       | 2.24          |
| (1,530) | 1:22:A:ARG:H  | 1:74:A:SER:CB | 10       | 2.24          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 7        | 2.24          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 18       | 2.24          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 3        | 2.24          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 4        | 2.24          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 19       | 2.24          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 5        | 2.24          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 3        | 2.24          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 3        | 2.23          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 17       | 2.23          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 11       | 2.23          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 7        | 2.23          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 18       | 2.23          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 14       | 2.23          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 1        | 2.23          |
| (1,713) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 14       | 2.23          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 11       | 2.23          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 16       | 2.23          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 10       | 2.23          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 19       | 2.23          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 6        | 2.23          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 20       | 2.23          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 9        | 2.23          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 5        | 2.23          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 2        | 2.23          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 15       | 2.23          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 11       | 2.23          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 18       | 2.23          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 8        | 2.23          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 4        | 2.23          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 7        | 2.23          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 15       | 2.23          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 1        | 2.22          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 20       | 2.22          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 14       | 2.22          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 20       | 2.22          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 8        | 2.22          |
| (1,625) | 1:37:A:CYS:CB | 1:87:A:SER:H  | 20       | 2.22          |
| (1,599) | 1:37:A:CYS:CB | 1:53:A:VAL:H  | 13       | 2.22          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 14       | 2.22          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 15       | 2.22          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 3        | 2.22          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 13       | 2.22          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 10       | 2.22          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 2        | 2.22          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 14       | 2.22          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 4        | 2.22          |
| (1,416) | 1:13:A:THR:H  | 1:99:A:LEU:CB | 16       | 2.22          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 3        | 2.22          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 5        | 2.22          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 1        | 2.22          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 19       | 2.21          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 9        | 2.21          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 10       | 2.21          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 2        | 2.21          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 14       | 2.21          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 9        | 2.21          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 9        | 2.21          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 18       | 2.21          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 10       | 2.21          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 20       | 2.2           |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 15       | 2.2           |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 13       | 2.2           |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 18       | 2.2           |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 6        | 2.2           |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 9        | 2.2           |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 10       | 2.2           |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 20       | 2.2           |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 6        | 2.2           |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 3        | 2.2           |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 7        | 2.2           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 7        | 2.2           |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 12       | 2.2           |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 20       | 2.2           |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 8        | 2.19          |
| (1,756) | 1:57:A:LEU:H  | 1:87:A:SER:CB | 14       | 2.19          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 17       | 2.19          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 19       | 2.19          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 15       | 2.19          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 15       | 2.19          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 13       | 2.19          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 11       | 2.19          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 13       | 2.19          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 18       | 2.19          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 4        | 2.19          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 12       | 2.19          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 6        | 2.19          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 19       | 2.19          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 7        | 2.19          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 19       | 2.18          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 5        | 2.18          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 10       | 2.18          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 15       | 2.18          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 16       | 2.18          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 16       | 2.18          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 1        | 2.18          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 14       | 2.18          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 7        | 2.18          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 11       | 2.18          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 3        | 2.18          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 6        | 2.18          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 2        | 2.18          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 12       | 2.18          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 17       | 2.18          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 5        | 2.18          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 8        | 2.18          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 18       | 2.18          |
| (1,813) | 1:84:A:ALA:H  | 1:99:A:LEU:CB | 10       | 2.17          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 11       | 2.17          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 11       | 2.17          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 16       | 2.17          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 17       | 2.17          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 3        | 2.17          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 16       | 2.17          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 13       | 2.17          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 15       | 2.17          |
| (1,736) | 1:56:A:SER:CB | 1:81:A:GLY:H  | 2        | 2.17          |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 2        | 2.17          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 17       | 2.17          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 15       | 2.17          |
| (1,583) | 1:33:A:LEU:H  | 1:99:A:LEU:CB | 12       | 2.17          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 15       | 2.17          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 18       | 2.17          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 6        | 2.17          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 4        | 2.17          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 12       | 2.17          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 20       | 2.17          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 6        | 2.17          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 18       | 2.17          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 6        | 2.17          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 1        | 2.17          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 14       | 2.17          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 7        | 2.16          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 18       | 2.16          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 19       | 2.16          |
| (1,762) | 1:59:A:THR:H  | 1:99:A:LEU:CB | 11       | 2.16          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 7        | 2.16          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 6        | 2.16          |
| (1,731) | 1:56:A:SER:CB | 1:72:A:LYS:H  | 19       | 2.16          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 2        | 2.16          |
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 6        | 2.16          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 8        | 2.16          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 14       | 2.16          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 3        | 2.16          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 16       | 2.16          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 17       | 2.16          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 2        | 2.16          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 10       | 2.16          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 14       | 2.16          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 13       | 2.16          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 17       | 2.16          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 17       | 2.15          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 16       | 2.15          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 11       | 2.15          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 12       | 2.15          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,699) | 1:47:A:SER:CB | 1:95:A:VAL:H  | 13       | 2.15          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 12       | 2.15          |
| (1,587) | 1:35:A:VAL:H  | 1:87:A:SER:CB | 16       | 2.15          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 5        | 2.15          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 4        | 2.15          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 19       | 2.15          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 12       | 2.15          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 12       | 2.15          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 7        | 2.14          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 12       | 2.14          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 9        | 2.14          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 3        | 2.14          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 4        | 2.14          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 7        | 2.14          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 7        | 2.14          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 16       | 2.14          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 11       | 2.14          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 15       | 2.14          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 8        | 2.14          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 10       | 2.14          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 2        | 2.13          |
| (1,776) | 1:64:A:ALA:H  | 1:87:A:SER:CB | 10       | 2.13          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 19       | 2.13          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 10       | 2.13          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 6        | 2.13          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 17       | 2.13          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 13       | 2.13          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 16       | 2.13          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 6        | 2.13          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 1        | 2.13          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 1        | 2.13          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 6        | 2.13          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 8        | 2.13          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 8        | 2.13          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 19       | 2.13          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 15       | 2.13          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 20       | 2.13          |
| (1,452) | 1:20:A:TYR:CB | 1:30:A:ILE:H  | 12       | 2.13          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 3        | 2.13          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 1        | 2.13          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 15       | 2.13          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 6        | 2.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 12       | 2.12          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 18       | 2.12          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 19       | 2.12          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 1        | 2.12          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 3        | 2.12          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 7        | 2.12          |
| (1,450) | 1:19:A:GLY:H  | 1:99:A:LEU:CB | 20       | 2.12          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 10       | 2.12          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 8        | 2.12          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 18       | 2.12          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 20       | 2.11          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 15       | 2.11          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 20       | 2.11          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 11       | 2.11          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 3        | 2.11          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 18       | 2.11          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 8        | 2.11          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 5        | 2.11          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 13       | 2.11          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 12       | 2.11          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 17       | 2.11          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 17       | 2.11          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 20       | 2.11          |
| (1,355) | 1:4:A:ILE:H   | 1:87:A:SER:CB | 14       | 2.11          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 1        | 2.1           |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 3        | 2.1           |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 10       | 2.1           |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 1        | 2.1           |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 14       | 2.1           |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 8        | 2.1           |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 2        | 2.1           |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 9        | 2.1           |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 11       | 2.1           |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 12       | 2.1           |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 1        | 2.1           |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 18       | 2.1           |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 1        | 2.1           |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 13       | 2.1           |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 1        | 2.1           |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 9        | 2.1           |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 13       | 2.1           |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 9        | 2.1           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,354) | 1:4:A:ILE:H   | 1:74:A:SER:CB | 14       | 2.1           |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 6        | 2.09          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 1        | 2.09          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 18       | 2.09          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 15       | 2.09          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 1        | 2.09          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 9        | 2.09          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 20       | 2.09          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 1        | 2.09          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 17       | 2.09          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 12       | 2.09          |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 12       | 2.09          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 7        | 2.09          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 15       | 2.09          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 12       | 2.09          |
| (1,568) | 1:30:A:ILE:H  | 1:74:A:SER:CB | 11       | 2.09          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 17       | 2.09          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 4        | 2.09          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 17       | 2.09          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 19       | 2.08          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 4        | 2.08          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 18       | 2.08          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 20       | 2.08          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 16       | 2.08          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 5        | 2.08          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 11       | 2.08          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 12       | 2.08          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 12       | 2.08          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 9        | 2.08          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 15       | 2.08          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 13       | 2.08          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 7        | 2.08          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 9        | 2.08          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 19       | 2.08          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 17       | 2.07          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 5        | 2.07          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 7        | 2.07          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 7        | 2.07          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 4        | 2.07          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 17       | 2.07          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 17       | 2.07          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 6        | 2.07          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 16       | 2.07          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 16       | 2.07          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 15       | 2.07          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 2        | 2.07          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 12       | 2.07          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 11       | 2.06          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 5        | 2.06          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 20       | 2.06          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 13       | 2.06          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 18       | 2.06          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 6        | 2.06          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 16       | 2.06          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 13       | 2.06          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 7        | 2.06          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 10       | 2.06          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 11       | 2.06          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 5        | 2.06          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 3        | 2.06          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 10       | 2.06          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 6        | 2.06          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 5        | 2.06          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 11       | 2.06          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 17       | 2.06          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 4        | 2.06          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 7        | 2.06          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 3        | 2.05          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 6        | 2.05          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 12       | 2.05          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 18       | 2.05          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 16       | 2.05          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 13       | 2.05          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 12       | 2.05          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 4        | 2.05          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 18       | 2.05          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 9        | 2.05          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 8        | 2.05          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 7        | 2.05          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 17       | 2.05          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 6        | 2.05          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 15       | 2.05          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 6        | 2.05          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 13       | 2.05          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 16       | 2.04          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 11       | 2.04          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 11       | 2.04          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 18       | 2.04          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 5        | 2.04          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 3        | 2.04          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 1        | 2.04          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 17       | 2.04          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 10       | 2.04          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 3        | 2.04          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 10       | 2.04          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 14       | 2.04          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 19       | 2.04          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 11       | 2.04          |
| (1,488) | 1:20:A:TYR:CB | 1:67:A:MET:H  | 2        | 2.04          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 8        | 2.04          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 1        | 2.04          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 8        | 2.04          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 16       | 2.04          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 12       | 2.04          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 14       | 2.04          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 9        | 2.03          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 14       | 2.03          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 20       | 2.03          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 3        | 2.03          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 1        | 2.03          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 3        | 2.03          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 8        | 2.03          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 16       | 2.03          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 8        | 2.03          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 4        | 2.03          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 13       | 2.03          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 5        | 2.03          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 1        | 2.03          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 3        | 2.03          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 3        | 2.03          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 2        | 2.03          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 17       | 2.03          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 9        | 2.02          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 6        | 2.02          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 9        | 2.02          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 18       | 2.02          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 17       | 2.02          |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 8        | 2.02          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 14       | 2.02          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 15       | 2.02          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 16       | 2.02          |
| (1,580) | 1:32:A:GLY:H  | 1:99:A:LEU:CB | 16       | 2.02          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 12       | 2.02          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 10       | 2.02          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 12       | 2.02          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 9        | 2.02          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 9        | 2.02          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 7        | 2.02          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 12       | 2.02          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 18       | 2.01          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 9        | 2.01          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 20       | 2.01          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 10       | 2.01          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 1        | 2.01          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 4        | 2.01          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 7        | 2.01          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 19       | 2.01          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 18       | 2.01          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 9        | 2.01          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 11       | 2.01          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 3        | 2.01          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 9        | 2.01          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 11       | 2.01          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 17       | 2.0           |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 16       | 2.0           |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 18       | 2.0           |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 8        | 2.0           |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 20       | 2.0           |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 4        | 2.0           |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 2        | 2.0           |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 5        | 2.0           |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 12       | 2.0           |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 8        | 2.0           |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 19       | 2.0           |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 15       | 2.0           |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 15       | 2.0           |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 10       | 2.0           |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 14       | 2.0           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 2        | 2.0           |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 1        | 2.0           |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 4        | 2.0           |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 11       | 2.0           |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 7        | 2.0           |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 9        | 2.0           |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 3        | 2.0           |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 7        | 2.0           |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 4        | 2.0           |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 6        | 2.0           |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 8        | 2.0           |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 15       | 2.0           |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 1        | 1.99          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 12       | 1.99          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 19       | 1.99          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 1        | 1.99          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 3        | 1.99          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 16       | 1.99          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 7        | 1.99          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 19       | 1.99          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 5        | 1.99          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 10       | 1.99          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 5        | 1.99          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 16       | 1.99          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 16       | 1.99          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 19       | 1.99          |
| (1,540) | 1:24:A:GLY:H  | 1:56:A:SER:CB | 3        | 1.99          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 1        | 1.99          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 20       | 1.99          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 16       | 1.99          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 2        | 1.98          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 13       | 1.98          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 17       | 1.98          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 5        | 1.98          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 14       | 1.98          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 10       | 1.98          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 15       | 1.98          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 5        | 1.98          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 3        | 1.98          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 19       | 1.98          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 15       | 1.98          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 18       | 1.98          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 1        | 1.98          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 5        | 1.97          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 13       | 1.97          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 6        | 1.97          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 7        | 1.97          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 8        | 1.97          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 13       | 1.97          |
| (1,742) | 1:56:A:SER:CB | 1:87:A:SER:H  | 5        | 1.97          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 13       | 1.97          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 8        | 1.97          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 16       | 1.97          |
| (1,606) | 1:37:A:CYS:CB | 1:60:A:ALA:H  | 20       | 1.97          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 6        | 1.97          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 7        | 1.97          |
| (1,579) | 1:32:A:GLY:H  | 1:87:A:SER:CB | 6        | 1.97          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 13       | 1.97          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 4        | 1.97          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 6        | 1.97          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 1        | 1.97          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 1        | 1.97          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 18       | 1.97          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 18       | 1.97          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 14       | 1.96          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 1        | 1.96          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 17       | 1.96          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 13       | 1.96          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 10       | 1.96          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 10       | 1.96          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 12       | 1.96          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 4        | 1.96          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 12       | 1.96          |
| (1,637) | 1:37:A:CYS:CB | 1:99:A:LEU:H  | 14       | 1.96          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 11       | 1.96          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 18       | 1.96          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 5        | 1.96          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 4        | 1.96          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 13       | 1.96          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 5        | 1.96          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 10       | 1.96          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 14       | 1.96          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 1        | 1.96          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 17       | 1.95          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 9        | 1.95          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 20       | 1.95          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 1        | 1.95          |
| (1,687) | 1:47:A:SER:CB | 1:83:A:VAL:H  | 14       | 1.95          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 14       | 1.95          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 5        | 1.95          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 10       | 1.95          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 5        | 1.95          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 9        | 1.95          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 12       | 1.95          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 19       | 1.95          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 6        | 1.95          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 8        | 1.95          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 17       | 1.94          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 5        | 1.94          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 5        | 1.94          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 11       | 1.94          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 19       | 1.94          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 2        | 1.94          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 8        | 1.94          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 10       | 1.94          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 15       | 1.94          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 20       | 1.94          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 11       | 1.94          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 1        | 1.93          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 18       | 1.93          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 13       | 1.93          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 12       | 1.93          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 3        | 1.93          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 10       | 1.93          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 8        | 1.93          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 18       | 1.93          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 9        | 1.93          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 7        | 1.93          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 20       | 1.93          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 3        | 1.93          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 1        | 1.93          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 12       | 1.93          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 9        | 1.93          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 3        | 1.93          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 20       | 1.92          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 16       | 1.92          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 8        | 1.92          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 6        | 1.92          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 16       | 1.92          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 3        | 1.92          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 12       | 1.92          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 9        | 1.92          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 19       | 1.92          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 13       | 1.92          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 16       | 1.92          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 4        | 1.92          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 16       | 1.92          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 6        | 1.92          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 10       | 1.92          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 5        | 1.92          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 9        | 1.91          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 4        | 1.91          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 13       | 1.91          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 3        | 1.91          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 5        | 1.91          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 19       | 1.91          |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 7        | 1.91          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 12       | 1.91          |
| (1,636) | 1:37:A:CYS:CB | 1:98:A:LEU:H  | 14       | 1.91          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 17       | 1.91          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 2        | 1.91          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 4        | 1.91          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 8        | 1.91          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 8        | 1.91          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 9        | 1.91          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 1        | 1.91          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 9        | 1.91          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 2        | 1.91          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 17       | 1.91          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 19       | 1.91          |
| (1,383) | 1:8:A:TYR:H   | 1:87:A:SER:CB | 5        | 1.91          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 11       | 1.9           |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 7        | 1.9           |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 11       | 1.9           |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 17       | 1.9           |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 3        | 1.9           |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 13       | 1.9           |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 17       | 1.9           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 7        | 1.9           |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 1        | 1.9           |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 3        | 1.9           |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 5        | 1.9           |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 13       | 1.9           |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 14       | 1.89          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 6        | 1.89          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 2        | 1.89          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 14       | 1.89          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 16       | 1.89          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 19       | 1.89          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 2        | 1.89          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 6        | 1.88          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 4        | 1.88          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 13       | 1.88          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 16       | 1.88          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 16       | 1.88          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 12       | 1.88          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 18       | 1.88          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 15       | 1.88          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 20       | 1.88          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 20       | 1.88          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 4        | 1.88          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 16       | 1.87          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 7        | 1.87          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 16       | 1.87          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 5        | 1.87          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 12       | 1.87          |
| (1,621) | 1:37:A:CYS:CB | 1:83:A:VAL:H  | 3        | 1.87          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 10       | 1.87          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 17       | 1.87          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 11       | 1.87          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 4        | 1.87          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 6        | 1.87          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 19       | 1.87          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 5        | 1.87          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 19       | 1.86          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 6        | 1.86          |
| (1,765) | 1:60:A:ALA:H  | 1:99:A:LEU:CB | 11       | 1.86          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 3        | 1.86          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 3        | 1.86          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 8        | 1.86          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 15       | 1.86          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 16       | 1.86          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 18       | 1.86          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 18       | 1.86          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 1        | 1.86          |
| (1,781) | 1:66:A:ILE:H  | 1:87:A:SER:CB | 7        | 1.85          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 4        | 1.85          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 11       | 1.85          |
| (1,740) | 1:56:A:SER:CB | 1:85:A:GLY:H  | 2        | 1.85          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 2        | 1.85          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 4        | 1.85          |
| (1,642) | 1:40:A:GLY:H  | 1:74:A:SER:CB | 5        | 1.85          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 20       | 1.85          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 14       | 1.85          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 1        | 1.85          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 16       | 1.85          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 16       | 1.85          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 7        | 1.85          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 18       | 1.85          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 1        | 1.84          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 14       | 1.84          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 5        | 1.84          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 4        | 1.84          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 5        | 1.84          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 9        | 1.84          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 11       | 1.84          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 18       | 1.84          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 15       | 1.84          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 14       | 1.84          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 4        | 1.84          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 15       | 1.83          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 15       | 1.83          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 9        | 1.83          |
| (1,768) | 1:61:A:PHE:H  | 1:99:A:LEU:CB | 4        | 1.83          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 19       | 1.83          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 4        | 1.83          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 15       | 1.83          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 5        | 1.83          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 2        | 1.83          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 18       | 1.83          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 12       | 1.83          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 6        | 1.83          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 5        | 1.83          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 5        | 1.83          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 18       | 1.83          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 11       | 1.82          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 11       | 1.82          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 10       | 1.82          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 17       | 1.82          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 5        | 1.82          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 12       | 1.82          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 1        | 1.82          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 3        | 1.82          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 20       | 1.82          |
| (1,342) | 1:2:A:ASP:H   | 1:87:A:SER:CB | 4        | 1.82          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 1        | 1.81          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 6        | 1.81          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 19       | 1.81          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 5        | 1.81          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 5        | 1.81          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 3        | 1.81          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 3        | 1.81          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 7        | 1.81          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 1        | 1.81          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 3        | 1.81          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 19       | 1.81          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 6        | 1.81          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 2        | 1.81          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 18       | 1.81          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 3        | 1.81          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 3        | 1.8           |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 6        | 1.8           |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 17       | 1.8           |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 6        | 1.8           |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 11       | 1.8           |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 15       | 1.8           |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 10       | 1.8           |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 3        | 1.8           |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 10       | 1.8           |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 15       | 1.8           |
| (1,494) | 1:20:A:TYR:CB | 1:73:A:ARG:H  | 12       | 1.8           |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 8        | 1.8           |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 2        | 1.79          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 9        | 1.79          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 19       | 1.79          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 4        | 1.79          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 15       | 1.79          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 20       | 1.79          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 6        | 1.79          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 9        | 1.79          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 4        | 1.79          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 6        | 1.79          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 13       | 1.79          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 18       | 1.79          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 8        | 1.79          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 19       | 1.79          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 5        | 1.79          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 1        | 1.79          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 2        | 1.79          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 4        | 1.79          |
| (1,556) | 1:28:A:SER:H  | 1:47:A:SER:CB | 10       | 1.79          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 4        | 1.79          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 4        | 1.79          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 17       | 1.79          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 8        | 1.79          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 7        | 1.79          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 12       | 1.79          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 5        | 1.79          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 9        | 1.79          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 15       | 1.78          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 7        | 1.78          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 14       | 1.78          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 9        | 1.78          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 8        | 1.78          |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 1        | 1.78          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 4        | 1.78          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 10       | 1.78          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 17       | 1.78          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 19       | 1.78          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 14       | 1.77          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 4        | 1.77          |
| (1,739) | 1:56:A:SER:CB | 1:84:A:ALA:H  | 2        | 1.77          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 2        | 1.77          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 12       | 1.77          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 2        | 1.77          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 4        | 1.77          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 15       | 1.77          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 14       | 1.77          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 10       | 1.77          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 15       | 1.76          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 8        | 1.76          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 7        | 1.76          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 6        | 1.76          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 14       | 1.76          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 15       | 1.76          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 10       | 1.76          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 8        | 1.76          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 4        | 1.76          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 15       | 1.76          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 12       | 1.76          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 12       | 1.76          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 3        | 1.75          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 10       | 1.75          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 4        | 1.75          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 4        | 1.75          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 3        | 1.75          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 16       | 1.75          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 6        | 1.75          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 4        | 1.75          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 14       | 1.75          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 19       | 1.75          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 3        | 1.75          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 12       | 1.75          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 16       | 1.74          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 8        | 1.74          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 2        | 1.74          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 5        | 1.74          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 9        | 1.74          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 17       | 1.74          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 11       | 1.74          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 17       | 1.74          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 19       | 1.74          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 15       | 1.74          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 9        | 1.74          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 13       | 1.74          |
| (1,745) | 1:56:A:SER:CB | 1:91:A:ILE:H  | 5        | 1.73          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 3        | 1.73          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 11       | 1.73          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 9        | 1.73          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 2        | 1.73          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 4        | 1.73          |
| (1,661) | 1:46:A:VAL:H  | 1:99:A:LEU:CB | 10       | 1.73          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 11       | 1.73          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 3        | 1.73          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 16       | 1.73          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 11       | 1.73          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 1        | 1.73          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 18       | 1.73          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 4        | 1.72          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 12       | 1.72          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 6        | 1.72          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 20       | 1.72          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 11       | 1.72          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 10       | 1.72          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 3        | 1.72          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 18       | 1.72          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 19       | 1.72          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 19       | 1.72          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 2        | 1.72          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 15       | 1.71          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 14       | 1.71          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 10       | 1.71          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 12       | 1.7           |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 11       | 1.7           |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 18       | 1.7           |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 13       | 1.7           |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 10       | 1.7           |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 13       | 1.7           |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 9        | 1.7           |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 19       | 1.7           |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 19       | 1.7           |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 19       | 1.7           |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 13       | 1.7           |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 20       | 1.7           |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 18       | 1.7           |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 14       | 1.7           |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 7        | 1.7           |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 8        | 1.7           |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 16       | 1.69          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 14       | 1.69          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 3        | 1.69          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 13       | 1.69          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 12       | 1.69          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 12       | 1.69          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 2        | 1.68          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 2        | 1.68          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 5        | 1.68          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 13       | 1.68          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 11       | 1.68          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 8        | 1.68          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 17       | 1.68          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 10       | 1.67          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 18       | 1.67          |
| (1,732) | 1:56:A:SER:CB | 1:73:A:ARG:H  | 13       | 1.67          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 9        | 1.67          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 1        | 1.67          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 7        | 1.67          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 2        | 1.67          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 16       | 1.67          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 9        | 1.67          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 7        | 1.67          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 11       | 1.67          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 9        | 1.66          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 16       | 1.66          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 10       | 1.66          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 20       | 1.66          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 3        | 1.66          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 11       | 1.66          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 2        | 1.66          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 2        | 1.66          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 13       | 1.66          |
| (1,597) | 1:37:A:CYS:CB | 1:49:A:ASP:H  | 16       | 1.66          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 16       | 1.66          |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 1        | 1.66          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 8        | 1.66          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 15       | 1.66          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 12       | 1.66          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 12       | 1.66          |
| (1,818) | 1:87:A:SER:CB | 1:98:A:LEU:H  | 11       | 1.65          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 11       | 1.65          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 12       | 1.65          |
| (1,758) | 1:58:A:PHE:H  | 1:87:A:SER:CB | 14       | 1.65          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 12       | 1.65          |
| (1,735) | 1:56:A:SER:CB | 1:80:A:ALA:H  | 2        | 1.65          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 12       | 1.65          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 20       | 1.65          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 4        | 1.65          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 10       | 1.65          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 20       | 1.65          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 18       | 1.65          |
| (1,514) | 1:20:A:TYR:CB | 1:92:A:LEU:H  | 14       | 1.65          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 11       | 1.65          |
| (1,459) | 1:20:A:TYR:CB | 1:39:A:ALA:H  | 9        | 1.65          |
| (1,410) | 1:12:A:VAL:H  | 1:87:A:SER:CB | 14       | 1.65          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 7        | 1.64          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 15       | 1.64          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 17       | 1.64          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 14       | 1.64          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 4        | 1.64          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 17       | 1.64          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 17       | 1.64          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 16       | 1.64          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 16       | 1.64          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 20       | 1.64          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 17       | 1.64          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 11       | 1.64          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 17       | 1.64          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 14       | 1.64          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 5        | 1.64          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 5        | 1.64          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 9        | 1.63          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 11       | 1.63          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 7        | 1.63          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 6        | 1.63          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 5        | 1.63          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 13       | 1.63          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 7        | 1.63          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 6        | 1.63          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 5        | 1.63          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 18       | 1.63          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 19       | 1.63          |
| (1,513) | 1:20:A:TYR:CB | 1:91:A:ILE:H  | 19       | 1.63          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 6        | 1.63          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 9        | 1.63          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 1        | 1.62          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 4        | 1.62          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 3        | 1.62          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 11       | 1.62          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 9        | 1.62          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 9        | 1.62          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 3        | 1.62          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 12       | 1.62          |
| (1,578) | 1:32:A:GLY:H  | 1:74:A:SER:CB | 11       | 1.62          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 4        | 1.62          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 10       | 1.62          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 14       | 1.61          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 3        | 1.61          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 6        | 1.61          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 20       | 1.61          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 1        | 1.61          |
| (1,753) | 1:56:A:SER:CB | 1:99:A:LEU:H  | 3        | 1.61          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 5        | 1.61          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 20       | 1.61          |
| (1,692) | 1:47:A:SER:CB | 1:88:A:LEU:H  | 4        | 1.61          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 10       | 1.61          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 18       | 1.61          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 16       | 1.61          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 3        | 1.6           |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 7        | 1.6           |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 5        | 1.6           |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 6        | 1.6           |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 7        | 1.6           |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 15       | 1.6           |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 11       | 1.6           |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 17       | 1.6           |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 16       | 1.6           |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 7        | 1.6           |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 3        | 1.6           |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 14       | 1.6           |
| (1,460) | 1:20:A:TYR:CB | 1:40:A:GLY:H  | 16       | 1.6           |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 12       | 1.6           |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 1        | 1.6           |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 9        | 1.6           |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 10       | 1.59          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 6        | 1.59          |
| (1,698) | 1:47:A:SER:CB | 1:94:A:LEU:H  | 17       | 1.59          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 18       | 1.59          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 2        | 1.59          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 14       | 1.59          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 8        | 1.59          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 5        | 1.59          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 5        | 1.58          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 9        | 1.58          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 3        | 1.58          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 20       | 1.58          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 13       | 1.58          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 2        | 1.58          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 18       | 1.58          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 14       | 1.58          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 4        | 1.57          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 16       | 1.57          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 16       | 1.57          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 19       | 1.57          |
| (1,738) | 1:56:A:SER:CB | 1:83:A:VAL:H  | 2        | 1.57          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 11       | 1.57          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 20       | 1.57          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 3        | 1.57          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 14       | 1.57          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 6        | 1.57          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 17       | 1.57          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 4        | 1.57          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 20       | 1.57          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 2        | 1.57          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 9        | 1.57          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 4        | 1.57          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 5        | 1.57          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 1        | 1.57          |
| (1,390) | 1:9:A:ALA:H   | 1:87:A:SER:CB | 14       | 1.57          |
| (1,817) | 1:87:A:SER:CB | 1:97:A:LEU:H  | 11       | 1.56          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 12       | 1.56          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 4        | 1.56          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 2        | 1.56          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 8        | 1.56          |
| (1,676) | 1:47:A:SER:CB | 1:68:A:GLY:H  | 18       | 1.56          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 6        | 1.56          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 20       | 1.56          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 1        | 1.56          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 15       | 1.55          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 16       | 1.55          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 12       | 1.55          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 6        | 1.55          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 7        | 1.55          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 2        | 1.55          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 1        | 1.55          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 3        | 1.55          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 3        | 1.55          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 5        | 1.55          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 9        | 1.54          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 14       | 1.54          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 13       | 1.54          |
| (1,778) | 1:65:A:THR:H  | 1:87:A:SER:CB | 10       | 1.54          |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 16       | 1.54          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 7        | 1.54          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 13       | 1.54          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 7        | 1.54          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 2        | 1.54          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 1        | 1.54          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 13       | 1.54          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 6        | 1.54          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 15       | 1.54          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 7        | 1.54          |
| (1,548) | 1:25:A:GLY:H  | 1:87:A:SER:CB | 9        | 1.54          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 1        | 1.54          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 11       | 1.54          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 7        | 1.54          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 15       | 1.53          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 8        | 1.53          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 14       | 1.53          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 7        | 1.53          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 20       | 1.53          |
| (1,586) | 1:35:A:VAL:H  | 1:74:A:SER:CB | 16       | 1.53          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 11       | 1.53          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 11       | 1.52          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 4        | 1.52          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 10       | 1.52          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 8        | 1.52          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 18       | 1.52          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 18       | 1.52          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 18       | 1.52          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 11       | 1.52          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 14       | 1.52          |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 16       | 1.52          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 8        | 1.52          |
| (1,350) | 1:4:A:ILE:H   | 1:20:A:TYR:CB | 10       | 1.52          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 1        | 1.51          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 17       | 1.51          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 3        | 1.51          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 15       | 1.51          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 3        | 1.51          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 18       | 1.51          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 19       | 1.51          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 13       | 1.51          |
| (1,658) | 1:44:A:TYR:H  | 1:99:A:LEU:CB | 10       | 1.51          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 1        | 1.51          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 8        | 1.51          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 13       | 1.51          |
| (1,607) | 1:37:A:CYS:CB | 1:61:A:PHE:H  | 4        | 1.51          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 14       | 1.51          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 16       | 1.51          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 7        | 1.51          |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 11       | 1.51          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 10       | 1.51          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 14       | 1.51          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 1        | 1.51          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 18       | 1.5           |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 15       | 1.5           |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 17       | 1.5           |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 16       | 1.5           |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 16       | 1.5           |
| (1,518) | 1:20:A:TYR:CB | 1:96:A:LEU:H  | 18       | 1.5           |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 14       | 1.5           |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 7        | 1.5           |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 4        | 1.49          |
| (1,791) | 1:70:A:ARG:H  | 1:87:A:SER:CB | 7        | 1.49          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 6        | 1.49          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 7        | 1.49          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 6        | 1.49          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 4        | 1.49          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 16       | 1.48          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 17       | 1.48          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 18       | 1.48          |
| (1,743) | 1:56:A:SER:H  | 1:87:A:SER:CB | 14       | 1.48          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 18       | 1.48          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 4        | 1.48          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 11       | 1.48          |
| (1,592) | 1:36:A:GLY:H  | 1:87:A:SER:CB | 16       | 1.48          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 15       | 1.48          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 13       | 1.48          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 7        | 1.48          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 8        | 1.48          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 6        | 1.47          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 1        | 1.47          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 7        | 1.47          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 7        | 1.47          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 14       | 1.47          |
| (1,662) | 1:47:A:SER:CB | 1:52:A:ASP:H  | 17       | 1.47          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 18       | 1.47          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 1        | 1.47          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 4        | 1.47          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 1        | 1.47          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 13       | 1.47          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 8        | 1.47          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 19       | 1.46          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 13       | 1.46          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 7        | 1.46          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 12       | 1.46          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 19       | 1.46          |
| (1,752) | 1:56:A:SER:CB | 1:98:A:LEU:H  | 11       | 1.46          |
| (1,749) | 1:56:A:SER:CB | 1:95:A:VAL:H  | 19       | 1.46          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 4        | 1.46          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 7        | 1.46          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 8        | 1.46          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 18       | 1.46          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 6        | 1.46          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 10       | 1.46          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 16       | 1.46          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 11       | 1.46          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 10       | 1.46          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 15       | 1.45          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 1        | 1.45          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 1        | 1.45          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 11       | 1.45          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 15       | 1.45          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 8        | 1.45          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 17       | 1.45          |
| (1,602) | 1:37:A:CYS:CB | 1:56:A:SER:H  | 13       | 1.45          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 3        | 1.45          |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 14       | 1.45          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 17       | 1.45          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 10       | 1.44          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 11       | 1.44          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 13       | 1.44          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 7        | 1.44          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 8        | 1.44          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 20       | 1.44          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 8        | 1.44          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 18       | 1.44          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 12       | 1.44          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 9        | 1.44          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 9        | 1.44          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 5        | 1.43          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 8        | 1.43          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 15       | 1.43          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 11       | 1.43          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 13       | 1.43          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 19       | 1.42          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 18       | 1.42          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 17       | 1.42          |
| (1,761) | 1:59:A:THR:H  | 1:87:A:SER:CB | 14       | 1.42          |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 10       | 1.42          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 11       | 1.42          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 14       | 1.42          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 19       | 1.42          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 9        | 1.41          |
| (1,764) | 1:60:A:ALA:H  | 1:87:A:SER:CB | 14       | 1.41          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 13       | 1.41          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 14       | 1.41          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 11       | 1.41          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 10       | 1.41          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 12       | 1.41          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 13       | 1.41          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 14       | 1.41          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 14       | 1.41          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 17       | 1.4           |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 7        | 1.4           |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 20       | 1.4           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 3        | 1.4           |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 3        | 1.4           |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 6        | 1.4           |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 19       | 1.4           |
| (1,639) | 1:39:A:ALA:H  | 1:87:A:SER:CB | 16       | 1.4           |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 1        | 1.4           |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 9        | 1.4           |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 17       | 1.4           |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 2        | 1.39          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 10       | 1.39          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 14       | 1.39          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 16       | 1.39          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 14       | 1.39          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 19       | 1.39          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 7        | 1.39          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 4        | 1.39          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 17       | 1.39          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 10       | 1.39          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 1        | 1.38          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 12       | 1.38          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 1        | 1.38          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 6        | 1.38          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 12       | 1.38          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 3        | 1.38          |
| (1,433) | 1:16:A:SER:H  | 1:87:A:SER:CB | 16       | 1.38          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 12       | 1.37          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 20       | 1.37          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 5        | 1.37          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 8        | 1.37          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 17       | 1.37          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 17       | 1.37          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 20       | 1.37          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 15       | 1.37          |
| (1,638) | 1:39:A:ALA:H  | 1:74:A:SER:CB | 16       | 1.37          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 18       | 1.37          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 1        | 1.37          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 13       | 1.37          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 13       | 1.37          |
| (1,364) | 1:6:A:PHE:H   | 1:20:A:TYR:CB | 16       | 1.37          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 9        | 1.37          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 7        | 1.36          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 6        | 1.36          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 9        | 1.36          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 15       | 1.36          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 4        | 1.36          |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 2        | 1.36          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 2        | 1.36          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 16       | 1.36          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 6        | 1.36          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 14       | 1.36          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 13       | 1.36          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 15       | 1.36          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 8        | 1.36          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 19       | 1.36          |
| (1,349) | 1:3:A:LEU:H   | 1:99:A:LEU:CB | 16       | 1.36          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 3        | 1.35          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 5        | 1.35          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 14       | 1.35          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 2        | 1.35          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 6        | 1.35          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 13       | 1.35          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 11       | 1.35          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 4        | 1.35          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 10       | 1.35          |
| (1,514) | 1:20:A:TYR:CB | 1:92:A:LEU:H  | 10       | 1.35          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 10       | 1.35          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 12       | 1.35          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 6        | 1.35          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 6        | 1.35          |
| (1,337) | 1:2:A:ASP:H   | 1:20:A:TYR:CB | 2        | 1.35          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 8        | 1.34          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 3        | 1.34          |
| (1,763) | 1:60:A:ALA:H  | 1:74:A:SER:CB | 2        | 1.34          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 15       | 1.34          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 10       | 1.34          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 17       | 1.34          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 2        | 1.34          |
| (1,376) | 1:7:A:GLY:H   | 1:87:A:SER:CB | 4        | 1.34          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 12       | 1.33          |
| (1,800) | 1:74:A:SER:CB | 1:93:A:ARG:H  | 20       | 1.33          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 7        | 1.33          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 13       | 1.33          |
| (1,700) | 1:47:A:SER:CB | 1:96:A:LEU:H  | 4        | 1.33          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 12       | 1.33          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 12       | 1.33          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 1        | 1.33          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 17       | 1.33          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 20       | 1.33          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 1        | 1.33          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 20       | 1.33          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 14       | 1.33          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 5        | 1.33          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 12       | 1.33          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 17       | 1.32          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 8        | 1.32          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 6        | 1.32          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 16       | 1.32          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 8        | 1.32          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 13       | 1.32          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 10       | 1.32          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 17       | 1.32          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 9        | 1.32          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 4        | 1.31          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 5        | 1.31          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 2        | 1.31          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 10       | 1.31          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 17       | 1.31          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 3        | 1.31          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 17       | 1.31          |
| (1,507) | 1:20:A:TYR:CB | 1:86:A:LEU:H  | 3        | 1.31          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 2        | 1.31          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 14       | 1.31          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 10       | 1.3           |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 12       | 1.3           |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 13       | 1.3           |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 4        | 1.3           |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 19       | 1.3           |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 16       | 1.3           |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 14       | 1.3           |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 18       | 1.29          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 7        | 1.29          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 19       | 1.29          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 6        | 1.29          |
| (1,444) | 1:18:A:PHE:H  | 1:87:A:SER:CB | 2        | 1.29          |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 19       | 1.29          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 3        | 1.28          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 13       | 1.28          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 2        | 1.28          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 10       | 1.28          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 11       | 1.28          |
| (1,612) | 1:37:A:CYS:CB | 1:66:A:ILE:H  | 19       | 1.28          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 15       | 1.28          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 5        | 1.27          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 8        | 1.27          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 15       | 1.27          |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 18       | 1.27          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 19       | 1.27          |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 10       | 1.27          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 8        | 1.27          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 4        | 1.27          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 15       | 1.27          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 6        | 1.26          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 14       | 1.26          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 9        | 1.26          |
| (1,784) | 1:67:A:MET:H  | 1:87:A:SER:CB | 7        | 1.26          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 13       | 1.26          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 2        | 1.26          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 14       | 1.26          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 15       | 1.26          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 13       | 1.26          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 19       | 1.26          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 15       | 1.26          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 15       | 1.26          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 7        | 1.26          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 14       | 1.26          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 17       | 1.26          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 7        | 1.25          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 12       | 1.25          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 2        | 1.25          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 1        | 1.25          |
| (1,631) | 1:37:A:CYS:CB | 1:93:A:ARG:H  | 20       | 1.25          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 12       | 1.25          |
| (1,485) | 1:20:A:TYR:CB | 1:64:A:ALA:H  | 2        | 1.25          |
| (1,439) | 1:17:A:ILE:H  | 1:87:A:SER:CB | 5        | 1.25          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 2        | 1.25          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 5        | 1.25          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 20       | 1.24          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 12       | 1.24          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 18       | 1.24          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 10       | 1.24          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 6        | 1.24          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 12       | 1.24          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 2        | 1.24          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 15       | 1.23          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 7        | 1.23          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 16       | 1.23          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 15       | 1.23          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 13       | 1.23          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 16       | 1.23          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 4        | 1.23          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 2        | 1.23          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 2        | 1.23          |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 4        | 1.23          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 8        | 1.23          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 10       | 1.23          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 3        | 1.23          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 2        | 1.23          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 8        | 1.23          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 11       | 1.22          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 17       | 1.22          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 18       | 1.22          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 5        | 1.22          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 7        | 1.22          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 1        | 1.22          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 13       | 1.22          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 12       | 1.22          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 10       | 1.22          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 19       | 1.22          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 15       | 1.22          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 19       | 1.21          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 4        | 1.21          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 8        | 1.21          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 4        | 1.21          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 11       | 1.21          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 18       | 1.21          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 13       | 1.2           |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 19       | 1.2           |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 3        | 1.2           |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 11       | 1.2           |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 17       | 1.2           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 3        | 1.2           |
| (1,581) | 1:33:A:LEU:H  | 1:74:A:SER:CB | 5        | 1.2           |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 13       | 1.2           |
| (1,547) | 1:25:A:GLY:H  | 1:74:A:SER:CB | 8        | 1.2           |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 10       | 1.2           |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 11       | 1.2           |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 13       | 1.19          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 9        | 1.19          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 15       | 1.19          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 10       | 1.19          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 6        | 1.19          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 4        | 1.19          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 3        | 1.19          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 8        | 1.18          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 1        | 1.18          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 17       | 1.18          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 6        | 1.18          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 13       | 1.18          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 15       | 1.18          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 2        | 1.18          |
| (1,575) | 1:31:A:ALA:H  | 1:99:A:LEU:CB | 6        | 1.18          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 11       | 1.18          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 14       | 1.18          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 18       | 1.17          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 9        | 1.17          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 9        | 1.17          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 1        | 1.17          |
| (1,715) | 1:51:A:ARG:H  | 1:87:A:SER:CB | 2        | 1.17          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 3        | 1.17          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 17       | 1.17          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 20       | 1.17          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 4        | 1.17          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 8        | 1.17          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 19       | 1.16          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 9        | 1.16          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 19       | 1.16          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 13       | 1.16          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 3        | 1.16          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 7        | 1.16          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 10       | 1.16          |
| (1,561) | 1:29:A:LEU:H  | 1:47:A:SER:CB | 20       | 1.16          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 5        | 1.16          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 18       | 1.16          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 18       | 1.16          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 9        | 1.16          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 19       | 1.16          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 20       | 1.15          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 10       | 1.15          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 11       | 1.15          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 7        | 1.15          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 12       | 1.15          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 17       | 1.15          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 6        | 1.15          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 20       | 1.15          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 4        | 1.15          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 2        | 1.15          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 4        | 1.14          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 11       | 1.14          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 8        | 1.14          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 12       | 1.14          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 12       | 1.14          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 10       | 1.14          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 8        | 1.14          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 7        | 1.14          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 15       | 1.14          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 11       | 1.14          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 20       | 1.14          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 14       | 1.13          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 20       | 1.13          |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 12       | 1.13          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 15       | 1.13          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 8        | 1.13          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 10       | 1.13          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 6        | 1.13          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 4        | 1.13          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 2        | 1.13          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 2        | 1.13          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 6        | 1.13          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 15       | 1.13          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 9        | 1.13          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 4        | 1.13          |
| (1,423) | 1:15:A:GLY:H  | 1:37:A:CYS:CB | 9        | 1.13          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 3        | 1.12          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 13       | 1.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 5        | 1.12          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 16       | 1.12          |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 17       | 1.12          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 9        | 1.12          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 11       | 1.12          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 6        | 1.12          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 2        | 1.12          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 17       | 1.11          |
| (1,822) | 1:89:A:MET:H  | 1:99:A:LEU:CB | 10       | 1.11          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 5        | 1.11          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 12       | 1.11          |
| (1,514) | 1:20:A:TYR:CB | 1:92:A:LEU:H  | 3        | 1.11          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 5        | 1.11          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 13       | 1.11          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 8        | 1.11          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 12       | 1.11          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 6        | 1.11          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 7        | 1.1           |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 8        | 1.1           |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 8        | 1.1           |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 20       | 1.1           |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 17       | 1.1           |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 13       | 1.1           |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 9        | 1.1           |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 8        | 1.1           |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 9        | 1.1           |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 2        | 1.1           |
| (1,127) | 1:37:A:CYS:H  | 1:47:A:SER:CB | 20       | 1.1           |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 12       | 1.09          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 1        | 1.09          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 19       | 1.09          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 13       | 1.09          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 5        | 1.09          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 1        | 1.08          |
| (1,780) | 1:66:A:ILE:H  | 1:74:A:SER:CB | 19       | 1.08          |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 8        | 1.08          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 18       | 1.08          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 2        | 1.08          |
| (1,628) | 1:37:A:CYS:CB | 1:90:A:MET:H  | 20       | 1.08          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 15       | 1.08          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 6        | 1.08          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 14       | 1.08          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 12       | 1.07          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 10       | 1.07          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 7        | 1.06          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 10       | 1.06          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 13       | 1.06          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 11       | 1.06          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 4        | 1.06          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 2        | 1.06          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 6        | 1.06          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 15       | 1.06          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 3        | 1.05          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 2        | 1.05          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 6        | 1.05          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 14       | 1.05          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 13       | 1.05          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 11       | 1.05          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 13       | 1.05          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 8        | 1.04          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 15       | 1.04          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 16       | 1.04          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 14       | 1.04          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 11       | 1.04          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 13       | 1.04          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 20       | 1.04          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 20       | 1.04          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 12       | 1.03          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 6        | 1.03          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 3        | 1.03          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 5        | 1.03          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 11       | 1.03          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 3        | 1.03          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 13       | 1.03          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 4        | 1.03          |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 3        | 1.03          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 6        | 1.03          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 12       | 1.03          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 3        | 1.03          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 18       | 1.03          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 17       | 1.02          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 1        | 1.02          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 7        | 1.02          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 1        | 1.02          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 17       | 1.02          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 20       | 1.01          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 9        | 1.01          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 3        | 1.01          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 20       | 1.01          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 9        | 1.01          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 12       | 1.01          |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 9        | 1.01          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 14       | 1.01          |
| (1,696) | 1:47:A:SER:CB | 1:92:A:LEU:H  | 4        | 1.01          |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 8        | 1.01          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 5        | 1.01          |
| (1,514) | 1:20:A:TYR:CB | 1:92:A:LEU:H  | 8        | 1.01          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 19       | 1.01          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 13       | 1.01          |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 8        | 1.01          |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 12       | 1.01          |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 20       | 1.01          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 10       | 1.0           |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 14       | 1.0           |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 17       | 1.0           |
| (1,769) | 1:62:A:PHE:H  | 1:74:A:SER:CB | 17       | 1.0           |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 14       | 1.0           |
| (1,697) | 1:47:A:SER:CB | 1:93:A:ARG:H  | 4        | 1.0           |
| (1,557) | 1:28:A:SER:H  | 1:56:A:SER:CB | 12       | 1.0           |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 19       | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 3        | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 4        | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 5        | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 6        | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 9        | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 10       | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 11       | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 13       | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 15       | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 16       | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 17       | 1.0           |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 18       | 1.0           |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 2        | 0.99          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 1        | 0.99          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 12       | 0.99          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 8        | 0.99          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 14       | 0.99          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 15       | 0.99          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 12       | 0.99          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 3        | 0.99          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 7        | 0.98          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 3        | 0.98          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 2        | 0.98          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 13       | 0.98          |
| (1,633) | 1:37:A:CYS:CB | 1:95:A:VAL:H  | 19       | 0.98          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 15       | 0.98          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 3        | 0.98          |
| (1,362) | 1:5:A:GLY:H   | 1:87:A:SER:CB | 5        | 0.98          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 13       | 0.97          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 20       | 0.97          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 18       | 0.97          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 9        | 0.97          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 8        | 0.97          |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 19       | 0.97          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 13       | 0.97          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 2        | 0.97          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 7        | 0.97          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 16       | 0.97          |
| (1,541) | 1:24:A:GLY:H  | 1:74:A:SER:CB | 12       | 0.97          |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 7        | 0.97          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 5        | 0.96          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 10       | 0.96          |
| (1,741) | 1:56:A:SER:CB | 1:86:A:LEU:H  | 2        | 0.96          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 16       | 0.96          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 6        | 0.96          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 8        | 0.96          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 12       | 0.96          |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 2        | 0.96          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 14       | 0.95          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 3        | 0.95          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 4        | 0.95          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 14       | 0.95          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 15       | 0.95          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 2        | 0.95          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 4        | 0.95          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 7        | 0.95          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 2        | 0.95          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 20       | 0.94          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 12       | 0.94          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 14       | 0.94          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 4        | 0.94          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 6        | 0.94          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 11       | 0.94          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 13       | 0.94          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 8        | 0.94          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 16       | 0.94          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 3        | 0.94          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 8        | 0.94          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 14       | 0.94          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 1        | 0.94          |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 19       | 0.94          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 4        | 0.93          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 12       | 0.93          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 13       | 0.93          |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 16       | 0.93          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 10       | 0.93          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 12       | 0.93          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 18       | 0.93          |
| (1,442) | 1:18:A:PHE:H  | 1:56:A:SER:CB | 20       | 0.93          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 11       | 0.92          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 19       | 0.92          |
| (1,770) | 1:62:A:PHE:H  | 1:87:A:SER:CB | 10       | 0.92          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 17       | 0.92          |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 15       | 0.92          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 15       | 0.92          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 4        | 0.92          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 16       | 0.92          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 18       | 0.92          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 18       | 0.92          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 20       | 0.92          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 11       | 0.91          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 3        | 0.91          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 3        | 0.91          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 9        | 0.91          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 2        | 0.9           |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 7        | 0.9           |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 5        | 0.9           |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 16       | 0.9           |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 4        | 0.9           |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 11       | 0.9           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 10       | 0.9           |
| (1,559) | 1:28:A:SER:H  | 1:99:A:LEU:CB | 6        | 0.9           |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 9        | 0.9           |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 16       | 0.9           |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 10       | 0.9           |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 1        | 0.9           |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 9        | 0.9           |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 19       | 0.9           |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 4        | 0.9           |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 3        | 0.89          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 8        | 0.89          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 12       | 0.89          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 15       | 0.89          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 6        | 0.89          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 12       | 0.89          |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 14       | 0.89          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 12       | 0.89          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 18       | 0.89          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 7        | 0.89          |
| (1,427) | 1:15:A:GLY:H  | 1:87:A:SER:CB | 20       | 0.89          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 15       | 0.89          |
| (1,348) | 1:3:A:LEU:H   | 1:87:A:SER:CB | 5        | 0.89          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 11       | 0.88          |
| (1,766) | 1:61:A:PHE:H  | 1:74:A:SER:CB | 8        | 0.88          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 17       | 0.88          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 19       | 0.88          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 2        | 0.88          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 1        | 0.88          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 6        | 0.88          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 7        | 0.88          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 14       | 0.88          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 20       | 0.88          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 1        | 0.88          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 1        | 0.87          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 11       | 0.87          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 9        | 0.87          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 17       | 0.87          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 10       | 0.87          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 4        | 0.87          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 14       | 0.87          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 14       | 0.87          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 1        | 0.86          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 2        | 0.86          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 18       | 0.86          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 20       | 0.86          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 2        | 0.86          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 20       | 0.86          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 15       | 0.86          |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 3        | 0.86          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 12       | 0.86          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 10       | 0.86          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 3        | 0.86          |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 14       | 0.86          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 7        | 0.85          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 2        | 0.85          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 14       | 0.85          |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 5        | 0.85          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 16       | 0.85          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 15       | 0.85          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 1        | 0.85          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 6        | 0.84          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 19       | 0.84          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 12       | 0.84          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 10       | 0.84          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 7        | 0.84          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 3        | 0.84          |
| (1,484) | 1:20:A:TYR:CB | 1:63:A:LEU:H  | 14       | 0.84          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 3        | 0.84          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 14       | 0.84          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 14       | 0.84          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 18       | 0.83          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 20       | 0.83          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 16       | 0.83          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 19       | 0.83          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 5        | 0.83          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 7        | 0.83          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 10       | 0.83          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 17       | 0.83          |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 17       | 0.83          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 4        | 0.83          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 19       | 0.82          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 3        | 0.82          |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 14       | 0.82          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 7        | 0.82          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 7        | 0.82          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 11       | 0.82          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 17       | 0.82          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 10       | 0.82          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 15       | 0.81          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 3        | 0.81          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 1        | 0.81          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 19       | 0.81          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 10       | 0.81          |
| (1,369) | 1:6:A:PHE:H   | 1:87:A:SER:CB | 13       | 0.81          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 18       | 0.8           |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 3        | 0.8           |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 18       | 0.8           |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 15       | 0.79          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 8        | 0.79          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 9        | 0.78          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 14       | 0.78          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 6        | 0.78          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 18       | 0.78          |
| (1,689) | 1:47:A:SER:CB | 1:85:A:GLY:H  | 5        | 0.78          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 8        | 0.78          |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 9        | 0.78          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 3        | 0.77          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 3        | 0.77          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 4        | 0.77          |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 7        | 0.77          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 5        | 0.77          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 18       | 0.77          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 13       | 0.77          |
| (1,296) | 1:66:A:ILE:H  | 1:99:A:LEU:CB | 1        | 0.77          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 4        | 0.76          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 10       | 0.76          |
| (1,627) | 1:37:A:CYS:CB | 1:89:A:MET:H  | 20       | 0.76          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 9        | 0.76          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 15       | 0.76          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 4        | 0.76          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 15       | 0.76          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 19       | 0.76          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 13       | 0.75          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 14       | 0.75          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 19       | 0.75          |
| (1,701) | 1:47:A:SER:CB | 1:97:A:LEU:H  | 6        | 0.75          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 10       | 0.75          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 15       | 0.74          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 2        | 0.74          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 6        | 0.74          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 17       | 0.74          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 14       | 0.74          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 10       | 0.74          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 5        | 0.74          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 5        | 0.73          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 4        | 0.73          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 19       | 0.73          |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 5        | 0.73          |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 7        | 0.73          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 11       | 0.73          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 3        | 0.73          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 7        | 0.73          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 17       | 0.73          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 5        | 0.73          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 16       | 0.73          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 16       | 0.72          |
| (1,717) | 1:52:A:ASP:H  | 1:87:A:SER:CB | 5        | 0.72          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 1        | 0.72          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 7        | 0.72          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 17       | 0.72          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 9        | 0.71          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 14       | 0.71          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 10       | 0.71          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 4        | 0.71          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 14       | 0.71          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 8        | 0.7           |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 15       | 0.7           |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 18       | 0.7           |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 15       | 0.7           |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 11       | 0.7           |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 14       | 0.7           |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 1        | 0.7           |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 2        | 0.69          |
| (1,814) | 1:85:A:GLY:H  | 1:99:A:LEU:CB | 10       | 0.69          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 3        | 0.69          |
| (1,695) | 1:47:A:SER:CB | 1:91:A:ILE:H  | 17       | 0.69          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 5        | 0.69          |
| (1,480) | 1:20:A:TYR:CB | 1:59:A:THR:H  | 19       | 0.69          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 13       | 0.69          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 18       | 0.69          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 1        | 0.68          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 15       | 0.68          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 9        | 0.68          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 12       | 0.68          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 1        | 0.68          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 10       | 0.68          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 20       | 0.68          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 10       | 0.68          |
| (1,514) | 1:20:A:TYR:CB | 1:92:A:LEU:H  | 6        | 0.68          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 11       | 0.68          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 8        | 0.68          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 12       | 0.67          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 9        | 0.67          |
| (1,644) | 1:40:A:GLY:H  | 1:99:A:LEU:CB | 16       | 0.67          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 16       | 0.67          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 20       | 0.67          |
| (1,514) | 1:20:A:TYR:CB | 1:92:A:LEU:H  | 16       | 0.67          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 13       | 0.67          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 4        | 0.66          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 12       | 0.66          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 13       | 0.66          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 20       | 0.66          |
| (1,505) | 1:20:A:TYR:CB | 1:84:A:ALA:H  | 1        | 0.66          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 14       | 0.65          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 4        | 0.65          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 18       | 0.65          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 1        | 0.65          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 9        | 0.65          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 15       | 0.65          |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 3        | 0.65          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 18       | 0.64          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 16       | 0.64          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 16       | 0.64          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 1        | 0.64          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 3        | 0.64          |
| (1,572) | 1:31:A:ALA:H  | 1:56:A:SER:CB | 16       | 0.64          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 17       | 0.64          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 12       | 0.64          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 15       | 0.64          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 7        | 0.63          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 17       | 0.63          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 13       | 0.63          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 2        | 0.63          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 2        | 0.63          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 15       | 0.63          |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 18       | 0.63          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 12       | 0.63          |
| (1,815) | 1:86:A:LEU:H  | 1:99:A:LEU:CB | 10       | 0.62          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 7        | 0.62          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 14       | 0.62          |
| (1,640) | 1:39:A:ALA:H  | 1:99:A:LEU:CB | 16       | 0.62          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 7        | 0.62          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 3        | 0.62          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 18       | 0.62          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 13       | 0.62          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 19       | 0.62          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 19       | 0.62          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 19       | 0.62          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 8        | 0.61          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 18       | 0.61          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 8        | 0.61          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 14       | 0.61          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 6        | 0.61          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 1        | 0.61          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 2        | 0.61          |
| (1,624) | 1:37:A:CYS:CB | 1:86:A:LEU:H  | 3        | 0.61          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 9        | 0.61          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 2        | 0.61          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 5        | 0.61          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 2        | 0.61          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 18       | 0.61          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 4        | 0.61          |
| (1,538) | 1:24:A:GLY:H  | 1:37:A:CYS:CB | 3        | 0.61          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 1        | 0.61          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 16       | 0.61          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 10       | 0.6           |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 17       | 0.6           |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 9        | 0.6           |
| (1,567) | 1:30:A:ILE:H  | 1:56:A:SER:CB | 20       | 0.6           |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 15       | 0.6           |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 3        | 0.6           |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 2        | 0.6           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 3        | 0.6           |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 16       | 0.59          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 9        | 0.59          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 13       | 0.59          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 13       | 0.59          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 17       | 0.59          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 7        | 0.59          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 12       | 0.59          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 7        | 0.59          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 8        | 0.59          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 14       | 0.59          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 17       | 0.59          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 4        | 0.58          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 16       | 0.58          |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 5        | 0.58          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 1        | 0.58          |
| (1,531) | 1:22:A:ARG:H  | 1:87:A:SER:CB | 20       | 0.58          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 15       | 0.57          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 6        | 0.57          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 18       | 0.57          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 20       | 0.57          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 3        | 0.57          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 6        | 0.56          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 10       | 0.56          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 3        | 0.56          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 16       | 0.56          |
| (1,767) | 1:61:A:PHE:H  | 1:87:A:SER:CB | 10       | 0.56          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 11       | 0.56          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 16       | 0.56          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 8        | 0.56          |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 12       | 0.56          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 12       | 0.55          |
| (1,593) | 1:36:A:GLY:H  | 1:99:A:LEU:CB | 16       | 0.55          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 10       | 0.55          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 5        | 0.55          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 1        | 0.54          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 11       | 0.54          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 6        | 0.54          |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 10       | 0.54          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 9        | 0.54          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 16       | 0.54          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 10       | 0.54          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 18       | 0.53          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 1        | 0.53          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 19       | 0.53          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 10       | 0.53          |
| (1,567) | 1:30:A:ILE:H  | 1:56:A:SER:CB | 8        | 0.53          |
| (1,567) | 1:30:A:ILE:H  | 1:56:A:SER:CB | 14       | 0.53          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 4        | 0.53          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 19       | 0.53          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 14       | 0.53          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 18       | 0.53          |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 6        | 0.53          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 14       | 0.52          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 17       | 0.52          |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 18       | 0.52          |
| (1,567) | 1:30:A:ILE:H  | 1:56:A:SER:CB | 1        | 0.52          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 2        | 0.52          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 10       | 0.52          |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 6        | 0.52          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 13       | 0.51          |
| (1,823) | 1:90:A:MET:H  | 1:99:A:LEU:CB | 20       | 0.51          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 4        | 0.51          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 7        | 0.51          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 5        | 0.51          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 15       | 0.51          |
| (1,705) | 1:48:A:ASN:H  | 1:87:A:SER:CB | 2        | 0.51          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 10       | 0.51          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 7        | 0.51          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 13       | 0.51          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 8        | 0.51          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 20       | 0.5           |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 2        | 0.5           |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 11       | 0.5           |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 19       | 0.5           |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 4        | 0.5           |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 3        | 0.5           |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 4        | 0.5           |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 6        | 0.5           |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 9        | 0.5           |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 11       | 0.5           |
| (1,417) | 1:14:A:PHE:H  | 1:37:A:CYS:CB | 17       | 0.5           |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 1        | 0.49          |
| (1,720) | 1:53:A:VAL:H  | 1:87:A:SER:CB | 5        | 0.49          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 8        | 0.49          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 12       | 0.49          |
| (1,525) | 1:21:A:LYS:H  | 1:56:A:SER:CB | 5        | 0.49          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 13       | 0.49          |
| (1,514) | 1:20:A:TYR:CB | 1:92:A:LEU:H  | 20       | 0.49          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 8        | 0.48          |
| (1,793) | 1:71:A:PHE:H  | 1:74:A:SER:CB | 15       | 0.48          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 8        | 0.48          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 19       | 0.48          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 10       | 0.48          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 17       | 0.48          |
| (1,554) | 1:26:A:VAL:H  | 1:87:A:SER:CB | 14       | 0.48          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 17       | 0.48          |
| (1,544) | 1:25:A:GLY:H  | 1:37:A:CYS:CB | 15       | 0.48          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 6        | 0.48          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 16       | 0.48          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 1        | 0.47          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 3        | 0.47          |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 20       | 0.47          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 9        | 0.47          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 12       | 0.47          |
| (1,577) | 1:32:A:GLY:H  | 1:56:A:SER:CB | 16       | 0.47          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 6        | 0.47          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 16       | 0.47          |
| (1,472) | 1:20:A:TYR:CB | 1:52:A:ASP:H  | 8        | 0.47          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 2        | 0.46          |
| (1,654) | 1:43:A:ALA:H  | 1:99:A:LEU:CB | 7        | 0.46          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 9        | 0.46          |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 2        | 0.46          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 17       | 0.45          |
| (1,789) | 1:69:A:VAL:H  | 1:87:A:SER:CB | 14       | 0.45          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 9        | 0.45          |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 4        | 0.45          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 5        | 0.45          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 9        | 0.45          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 2        | 0.45          |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 4        | 0.45          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 11       | 0.45          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 6        | 0.44          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 4        | 0.44          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 7        | 0.44          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 6        | 0.44          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 1        | 0.44          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 18       | 0.44          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 17       | 0.44          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 9        | 0.44          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 13       | 0.44          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 10       | 0.44          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 20       | 0.44          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 7        | 0.44          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 7        | 0.44          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 13       | 0.44          |
| (1,429) | 1:16:A:SER:H  | 1:37:A:CYS:CB | 16       | 0.44          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 5        | 0.44          |
| (1,744) | 1:56:A:SER:CB | 1:88:A:LEU:H  | 19       | 0.43          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 12       | 0.43          |
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 12       | 0.43          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 12       | 0.43          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 12       | 0.43          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 14       | 0.43          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 13       | 0.42          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 12       | 0.42          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 15       | 0.42          |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 3        | 0.42          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 15       | 0.42          |
| (1,558) | 1:28:A:SER:H  | 1:74:A:SER:CB | 12       | 0.42          |
| (1,535) | 1:23:A:ARG:H  | 1:56:A:SER:CB | 14       | 0.42          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 20       | 0.41          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 9        | 0.41          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 7        | 0.41          |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 13       | 0.41          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 11       | 0.41          |
| (1,737) | 1:56:A:SER:CB | 1:82:A:LEU:H  | 2        | 0.41          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 8        | 0.41          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 18       | 0.41          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 9        | 0.41          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 19       | 0.41          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 6        | 0.4           |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 5        | 0.4           |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 12       | 0.4           |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 5        | 0.4           |
| (1,750) | 1:56:A:SER:CB | 1:96:A:LEU:H  | 19       | 0.4           |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 5        | 0.4           |
| (1,664) | 1:47:A:SER:CB | 1:54:A:LYS:H  | 6        | 0.4           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 1        | 0.4           |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 8        | 0.4           |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 5        | 0.4           |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 11       | 0.39          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 10       | 0.39          |
| (1,645) | 1:41:A:TYR:H  | 1:56:A:SER:CB | 10       | 0.39          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 6        | 0.39          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 15       | 0.39          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 11       | 0.39          |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 10       | 0.39          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 1        | 0.38          |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 15       | 0.38          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 15       | 0.38          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 9        | 0.38          |
| (1,585) | 1:35:A:VAL:H  | 1:56:A:SER:CB | 16       | 0.38          |
| (1,567) | 1:30:A:ILE:H  | 1:56:A:SER:CB | 18       | 0.38          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 18       | 0.38          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 16       | 0.38          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 15       | 0.38          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 1        | 0.38          |
| (1,422) | 1:14:A:PHE:H  | 1:99:A:LEU:CB | 11       | 0.38          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 16       | 0.37          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 3        | 0.37          |
| (1,461) | 1:20:A:TYR:CB | 1:41:A:TYR:H  | 19       | 0.37          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 5        | 0.36          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 15       | 0.36          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 11       | 0.36          |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 7        | 0.36          |
| (1,609) | 1:37:A:CYS:CB | 1:63:A:LEU:H  | 10       | 0.36          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 16       | 0.36          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 14       | 0.36          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 12       | 0.36          |
| (1,477) | 1:20:A:TYR:H  | 1:56:A:SER:CB | 2        | 0.36          |
| (1,415) | 1:13:A:THR:H  | 1:87:A:SER:CB | 14       | 0.36          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 4        | 0.35          |
| (4,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:N  | 8        | 0.35          |
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 10       | 0.35          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 18       | 0.35          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 2        | 0.35          |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 11       | 0.35          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 14       | 0.35          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 9        | 0.35          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,648) | 1:41:A:TYR:H  | 1:99:A:LEU:CB | 2        | 0.35          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 5        | 0.35          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 16       | 0.35          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 2        | 0.35          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 7        | 0.35          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 1        | 0.35          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 17       | 0.35          |
| (1,821) | 1:88:A:LEU:H  | 1:99:A:LEU:CB | 13       | 0.34          |
| (1,746) | 1:56:A:SER:CB | 1:92:A:LEU:H  | 19       | 0.34          |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 2        | 0.34          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 7        | 0.34          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 4        | 0.34          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 11       | 0.34          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 8        | 0.34          |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 8        | 0.33          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 2        | 0.33          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 13       | 0.33          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 2        | 0.33          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 13       | 0.33          |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 1        | 0.33          |
| (1,226) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 17       | 0.33          |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 19       | 0.33          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 16       | 0.32          |
| (1,798) | 1:74:A:SER:CB | 1:91:A:ILE:H  | 3        | 0.32          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 1        | 0.32          |
| (1,590) | 1:36:A:GLY:H  | 1:56:A:SER:CB | 16       | 0.32          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 18       | 0.32          |
| (1,499) | 1:20:A:TYR:CB | 1:77:A:ILE:H  | 1        | 0.32          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 20       | 0.32          |
| (1,226) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 13       | 0.32          |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 20       | 0.32          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 3        | 0.31          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 4        | 0.31          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 17       | 0.31          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 3        | 0.31          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 11       | 0.31          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 20       | 0.31          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 2        | 0.31          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 13       | 0.31          |
| (4,11)  | 1:38:A:LEU:O  | 1:42:A:GLY:N  | 20       | 0.31          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 18       | 0.31          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 2        | 0.31          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,796) | 1:74:A:SER:CB | 1:89:A:MET:H  | 19       | 0.31          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 16       | 0.31          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 13       | 0.31          |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 9        | 0.31          |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 14       | 0.31          |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 15       | 0.31          |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 2        | 0.31          |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 20       | 0.31          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 11       | 0.3           |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 20       | 0.3           |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 11       | 0.3           |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 13       | 0.3           |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 15       | 0.3           |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 16       | 0.3           |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 18       | 0.3           |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 3        | 0.3           |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 4        | 0.3           |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 12       | 0.3           |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 13       | 0.3           |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 14       | 0.3           |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 16       | 0.3           |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 17       | 0.3           |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 11       | 0.3           |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 12       | 0.3           |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 17       | 0.3           |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 10       | 0.3           |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 12       | 0.3           |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 7        | 0.3           |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 11       | 0.3           |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 15       | 0.3           |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 16       | 0.3           |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 7        | 0.3           |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 14       | 0.3           |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 15       | 0.3           |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 19       | 0.3           |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 20       | 0.3           |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 16       | 0.3           |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 7        | 0.3           |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 15       | 0.3           |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 6        | 0.3           |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 11       | 0.3           |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 12       | 0.3           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 11       | 0.3           |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 12       | 0.3           |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 13       | 0.3           |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 18       | 0.3           |
| (4,3)   | 1:13:A:THR:O  | 1:17:A:ILE:N  | 7        | 0.3           |
| (1,721) | 1:53:A:VAL:H  | 1:99:A:LEU:CB | 6        | 0.3           |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 16       | 0.3           |
| (1,693) | 1:47:A:SER:CB | 1:89:A:MET:H  | 4        | 0.3           |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 20       | 0.3           |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 17       | 0.3           |
| (1,564) | 1:29:A:LEU:H  | 1:87:A:SER:CB | 6        | 0.3           |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 18       | 0.3           |
| (1,514) | 1:20:A:TYR:CB | 1:92:A:LEU:H  | 7        | 0.3           |
| (1,441) | 1:18:A:PHE:H  | 1:37:A:CYS:CB | 9        | 0.3           |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 4        | 0.3           |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 6        | 0.3           |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 8        | 0.3           |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 18       | 0.3           |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 4        | 0.3           |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 5        | 0.3           |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 7        | 0.3           |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 10       | 0.3           |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 15       | 0.3           |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 16       | 0.3           |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 18       | 0.3           |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 19       | 0.3           |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 16       | 0.29          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 5        | 0.29          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 20       | 0.29          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 2        | 0.29          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 5        | 0.29          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 6        | 0.29          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 10       | 0.29          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 11       | 0.29          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 20       | 0.29          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 2        | 0.29          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 19       | 0.29          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 9        | 0.29          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 1        | 0.29          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 7        | 0.29          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 3        | 0.29          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 8        | 0.29          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 19       | 0.29          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 2        | 0.29          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 4        | 0.29          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 19       | 0.29          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 3        | 0.29          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 19       | 0.29          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 5        | 0.29          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 15       | 0.29          |
| (4,10)  | 1:39:A:ALA:O  | 1:43:A:ALA:N  | 7        | 0.29          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 13       | 0.29          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 19       | 0.29          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 5        | 0.29          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 11       | 0.29          |
| (1,747) | 1:56:A:SER:CB | 1:93:A:ARG:H  | 5        | 0.29          |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 20       | 0.29          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 4        | 0.29          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 2        | 0.29          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 2        | 0.29          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 17       | 0.29          |
| (4,109) | 1:53:A:VAL:O  | 1:57:A:LEU:H  | 13       | 0.28          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 1        | 0.28          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 10       | 0.28          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 19       | 0.28          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 1        | 0.28          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 9        | 0.28          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 18       | 0.28          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 15       | 0.28          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 8        | 0.28          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 13       | 0.28          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 19       | 0.28          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 1        | 0.28          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 8        | 0.28          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 13       | 0.28          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 18       | 0.28          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 2        | 0.28          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 15       | 0.28          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 14       | 0.28          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 17       | 0.28          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 1        | 0.28          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 5        | 0.28          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 14       | 0.28          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 17       | 0.28          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 20       | 0.28          |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 1        | 0.28          |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 4        | 0.28          |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 18       | 0.28          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 7        | 0.28          |
| (4,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:N  | 6        | 0.28          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 1        | 0.28          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 9        | 0.28          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 10       | 0.28          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 13       | 0.28          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 17       | 0.28          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 4        | 0.28          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 6        | 0.28          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 1        | 0.28          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 12       | 0.28          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 7        | 0.28          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 10       | 0.28          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 12       | 0.28          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 16       | 0.28          |
| (4,10)  | 1:39:A:ALA:O  | 1:43:A:ALA:N  | 12       | 0.28          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 5        | 0.28          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 14       | 0.28          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 15       | 0.28          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 12       | 0.28          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 15       | 0.28          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 17       | 0.28          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 18       | 0.28          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 16       | 0.28          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 5        | 0.28          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 7        | 0.28          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 3        | 0.28          |
| (1,645) | 1:41:A:TYR:H  | 1:56:A:SER:CB | 16       | 0.28          |
| (1,536) | 1:23:A:ARG:H  | 1:74:A:SER:CB | 12       | 0.28          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 12       | 0.28          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 5        | 0.28          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 9        | 0.28          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 12       | 0.28          |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 13       | 0.28          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 3        | 0.27          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 4        | 0.27          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 9        | 0.27          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 14       | 0.27          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 7        | 0.27          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 8        | 0.27          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 12       | 0.27          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 4        | 0.27          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 6        | 0.27          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 17       | 0.27          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 3        | 0.27          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 5        | 0.27          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 4        | 0.27          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 9        | 0.27          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 14       | 0.27          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 20       | 0.27          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 9        | 0.27          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 6        | 0.27          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 6        | 0.27          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 19       | 0.27          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 4        | 0.27          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 8        | 0.27          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 17       | 0.27          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 6        | 0.27          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 9        | 0.27          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 15       | 0.27          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 19       | 0.27          |
| (4,3)   | 1:13:A:THR:O  | 1:17:A:ILE:N  | 16       | 0.27          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 15       | 0.27          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 19       | 0.27          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 8        | 0.27          |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 19       | 0.27          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 4        | 0.27          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 15       | 0.27          |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 5        | 0.27          |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 17       | 0.27          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 4        | 0.26          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 17       | 0.26          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 3        | 0.26          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 17       | 0.26          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 2        | 0.26          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 6        | 0.26          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 8        | 0.26          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 15       | 0.26          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 6        | 0.26          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 7        | 0.26          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Model ID | Violation (Å) |
|---------|--------------|---------------|----------|---------------|
| (4,39)  | 1:85:A:GLY:O | 1:89:A:MET:N  | 9        | 0.26          |
| (4,38)  | 1:86:A:LEU:O | 1:90:A:MET:N  | 1        | 0.26          |
| (4,38)  | 1:86:A:LEU:O | 1:90:A:MET:N  | 2        | 0.26          |
| (4,37)  | 1:87:A:SER:O | 1:91:A:ILE:N  | 6        | 0.26          |
| (4,37)  | 1:87:A:SER:O | 1:91:A:ILE:N  | 7        | 0.26          |
| (4,37)  | 1:87:A:SER:O | 1:91:A:ILE:N  | 10       | 0.26          |
| (4,36)  | 1:88:A:LEU:O | 1:92:A:LEU:N  | 6        | 0.26          |
| (4,30)  | 1:56:A:SER:O | 1:60:A:ALA:N  | 5        | 0.26          |
| (4,29)  | 1:57:A:LEU:O | 1:61:A:PHE:N  | 1        | 0.26          |
| (4,29)  | 1:57:A:LEU:O | 1:61:A:PHE:N  | 16       | 0.26          |
| (4,28)  | 1:58:A:PHE:O | 1:62:A:PHE:N  | 12       | 0.26          |
| (4,28)  | 1:58:A:PHE:O | 1:62:A:PHE:N  | 18       | 0.26          |
| (4,27)  | 1:59:A:THR:O | 1:63:A:LEU:N  | 5        | 0.26          |
| (4,26)  | 1:60:A:ALA:O | 1:64:A:ALA:N  | 6        | 0.26          |
| (4,26)  | 1:60:A:ALA:O | 1:64:A:ALA:N  | 7        | 0.26          |
| (4,26)  | 1:60:A:ALA:O | 1:64:A:ALA:N  | 12       | 0.26          |
| (4,25)  | 1:61:A:PHE:O | 1:65:A:THR:N  | 3        | 0.26          |
| (4,25)  | 1:61:A:PHE:O | 1:65:A:THR:N  | 5        | 0.26          |
| (4,25)  | 1:61:A:PHE:O | 1:65:A:THR:N  | 17       | 0.26          |
| (4,21)  | 1:28:A:SER:O | 1:32:A:GLY:N  | 20       | 0.26          |
| (4,18)  | 1:31:A:ALA:O | 1:35:A:VAL:N  | 2        | 0.26          |
| (4,18)  | 1:31:A:ALA:O | 1:35:A:VAL:N  | 8        | 0.26          |
| (4,18)  | 1:31:A:ALA:O | 1:35:A:VAL:N  | 16       | 0.26          |
| (4,17)  | 1:32:A:GLY:O | 1:36:A:GLY:N  | 12       | 0.26          |
| (4,17)  | 1:32:A:GLY:O | 1:36:A:GLY:N  | 13       | 0.26          |
| (4,14)  | 1:35:A:VAL:O | 1:39:A:ALA:N  | 5        | 0.26          |
| (4,13)  | 1:36:A:GLY:O | 1:40:A:GLY:N  | 18       | 0.26          |
| (4,7)   | 1:9:A:ALA:O  | 1:13:A:THR:N  | 4        | 0.26          |
| (4,7)   | 1:9:A:ALA:O  | 1:13:A:THR:N  | 7        | 0.26          |
| (4,6)   | 1:10:A:ALA:O | 1:14:A:PHE:N  | 1        | 0.26          |
| (4,6)   | 1:10:A:ALA:O | 1:14:A:PHE:N  | 4        | 0.26          |
| (4,6)   | 1:10:A:ALA:O | 1:14:A:PHE:N  | 6        | 0.26          |
| (4,6)   | 1:10:A:ALA:O | 1:14:A:PHE:N  | 9        | 0.26          |
| (4,6)   | 1:10:A:ALA:O | 1:14:A:PHE:N  | 10       | 0.26          |
| (4,5)   | 1:11:A:LEU:O | 1:15:A:GLY:N  | 4        | 0.26          |
| (4,2)   | 1:14:A:PHE:O | 1:18:A:PHE:N  | 6        | 0.26          |
| (3,22)  | 1:64:A:ALA:O | 1:68:A:GLY:H  | 7        | 0.26          |
| (1,821) | 1:88:A:LEU:H | 1:99:A:LEU:CB | 1        | 0.26          |
| (1,421) | 1:14:A:PHE:H | 1:87:A:SER:CB | 1        | 0.26          |
| (4,44)  | 1:80:A:ALA:O | 1:84:A:ALA:N  | 11       | 0.25          |
| (4,44)  | 1:80:A:ALA:O | 1:84:A:ALA:N  | 20       | 0.25          |
| (4,42)  | 1:82:A:LEU:O | 1:86:A:LEU:N  | 1        | 0.25          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 6        | 0.25          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 8        | 0.25          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 13       | 0.25          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 16       | 0.25          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 7        | 0.25          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 13       | 0.25          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 5        | 0.25          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 10       | 0.25          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 18       | 0.25          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 13       | 0.25          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 16       | 0.25          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 19       | 0.25          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 6        | 0.25          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 9        | 0.25          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 11       | 0.25          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 10       | 0.25          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 13       | 0.25          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 17       | 0.25          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 8        | 0.25          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 1        | 0.25          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 12       | 0.25          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 8        | 0.25          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 10       | 0.25          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 8        | 0.25          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 3        | 0.25          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 2        | 0.25          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 3        | 0.25          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 4        | 0.25          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 8        | 0.25          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 14       | 0.25          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 20       | 0.25          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 8        | 0.25          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 19       | 0.25          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 3        | 0.25          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 5        | 0.25          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 13       | 0.25          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 18       | 0.25          |
| (3,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 11       | 0.25          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 3        | 0.25          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 20       | 0.25          |
| (1,617) | 1:37:A:CYS:CB | 1:71:A:PHE:H  | 16       | 0.25          |
| (1,562) | 1:29:A:LEU:H  | 1:56:A:SER:CB | 11       | 0.25          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 7        | 0.25          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 13       | 0.25          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 3        | 0.25          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 15       | 0.25          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 20       | 0.25          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 10       | 0.24          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 18       | 0.24          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 19       | 0.24          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 16       | 0.24          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 14       | 0.24          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 3        | 0.24          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 2        | 0.24          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 17       | 0.24          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 3        | 0.24          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 6        | 0.24          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 4        | 0.24          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 8        | 0.24          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 10       | 0.24          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 12       | 0.24          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 20       | 0.24          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 11       | 0.24          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 3        | 0.24          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 17       | 0.24          |
| (4,16)  | 1:33:A:LEU:O  | 1:37:A:CYS:N  | 4        | 0.24          |
| (4,16)  | 1:33:A:LEU:O  | 1:37:A:CYS:N  | 15       | 0.24          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 7        | 0.24          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 1        | 0.24          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 10       | 0.24          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 20       | 0.24          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 6        | 0.24          |
| (4,11)  | 1:38:A:LEU:O  | 1:42:A:GLY:N  | 10       | 0.24          |
| (4,11)  | 1:38:A:LEU:O  | 1:42:A:GLY:N  | 19       | 0.24          |
| (4,10)  | 1:39:A:ALA:O  | 1:43:A:ALA:N  | 16       | 0.24          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 15       | 0.24          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 16       | 0.24          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 7        | 0.24          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 8        | 0.24          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 14       | 0.24          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 5        | 0.24          |
| (1,481) | 1:20:A:TYR:CB | 1:60:A:ALA:H  | 19       | 0.24          |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 11       | 0.24          |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 14       | 0.24          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 14       | 0.23          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 5        | 0.23          |
| (4,41)  | 1:83:A:VAL:O  | 1:87:A:SER:N  | 12       | 0.23          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 10       | 0.23          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 12       | 0.23          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 4        | 0.23          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 15       | 0.23          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 19       | 0.23          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 10       | 0.23          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 12       | 0.23          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 15       | 0.23          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 8        | 0.23          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 18       | 0.23          |
| (4,28)  | 1:58:A:PHE:O  | 1:62:A:PHE:N  | 8        | 0.23          |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 6        | 0.23          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 9        | 0.23          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 10       | 0.23          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 4        | 0.23          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 12       | 0.23          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 14       | 0.23          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 16       | 0.23          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 3        | 0.23          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 2        | 0.23          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 7        | 0.23          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 17       | 0.23          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 19       | 0.23          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 7        | 0.23          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 19       | 0.23          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 2        | 0.23          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 3        | 0.23          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 1        | 0.23          |
| (4,4)   | 1:12:A:VAL:O  | 1:16:A:SER:N  | 7        | 0.23          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 4        | 0.23          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 9        | 0.23          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 11       | 0.23          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 12       | 0.23          |
| (3,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 15       | 0.23          |
| (3,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 18       | 0.23          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 8        | 0.23          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 17       | 0.23          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 9        | 0.23          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 17       | 0.23          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 16       | 0.23          |
| (1,645) | 1:41:A:TYR:H  | 1:56:A:SER:CB | 1        | 0.23          |
| (1,500) | 1:20:A:TYR:CB | 1:78:A:MET:H  | 7        | 0.23          |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 10       | 0.23          |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 3        | 0.23          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 13       | 0.22          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 16       | 0.22          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 17       | 0.22          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 8        | 0.22          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 19       | 0.22          |
| (4,33)  | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 11       | 0.22          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 2        | 0.22          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 7        | 0.22          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 9        | 0.22          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 14       | 0.22          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 16       | 0.22          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 19       | 0.22          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 7        | 0.22          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 13       | 0.22          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 20       | 0.22          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 2        | 0.22          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 16       | 0.22          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 19       | 0.22          |
| (4,24)  | 1:62:A:PHE:O  | 1:66:A:ILE:N  | 10       | 0.22          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 19       | 0.22          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 20       | 0.22          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 5        | 0.22          |
| (4,16)  | 1:33:A:LEU:O  | 1:37:A:CYS:N  | 18       | 0.22          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 13       | 0.22          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 19       | 0.22          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 4        | 0.22          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 12       | 0.22          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 13       | 0.22          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 16       | 0.22          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 20       | 0.22          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 14       | 0.22          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 11       | 0.22          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 8        | 0.22          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 3        | 0.22          |
| (4,4)   | 1:12:A:VAL:O  | 1:16:A:SER:N  | 8        | 0.22          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 1        | 0.22          |
| (3,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 13       | 0.22          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 6        | 0.22          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 5        | 0.22          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 11       | 0.22          |
| (1,440) | 1:17:A:ILE:H  | 1:99:A:LEU:CB | 13       | 0.22          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 3        | 0.22          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 4        | 0.22          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 11       | 0.22          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 4        | 0.22          |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 12       | 0.22          |
| (4,110) | 1:53:A:VAL:O  | 1:57:A:LEU:N  | 13       | 0.21          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 5        | 0.21          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 15       | 0.21          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 18       | 0.21          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 15       | 0.21          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 5        | 0.21          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 2        | 0.21          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 16       | 0.21          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 10       | 0.21          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 1        | 0.21          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 11       | 0.21          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 13       | 0.21          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 17       | 0.21          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 14       | 0.21          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 2        | 0.21          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 5        | 0.21          |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 3        | 0.21          |
| (4,24)  | 1:62:A:PHE:O  | 1:66:A:ILE:N  | 11       | 0.21          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 4        | 0.21          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 7        | 0.21          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 8        | 0.21          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 10       | 0.21          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 11       | 0.21          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 13       | 0.21          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 15       | 0.21          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 16       | 0.21          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 14       | 0.21          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 15       | 0.21          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 4        | 0.21          |
| (4,18)  | 1:31:A:ALA:O  | 1:35:A:VAL:N  | 18       | 0.21          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 1        | 0.21          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 1        | 0.21          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 10       | 0.21          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 13       | 0.21          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 16       | 0.21          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 7        | 0.21          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 10       | 0.21          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 11       | 0.21          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 6        | 0.21          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 12       | 0.21          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 5        | 0.21          |
| (1,645) | 1:41:A:TYR:H  | 1:56:A:SER:CB | 7        | 0.21          |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 1        | 0.21          |
| (1,567) | 1:30:A:ILE:H  | 1:56:A:SER:CB | 9        | 0.21          |
| (1,567) | 1:30:A:ILE:H  | 1:56:A:SER:CB | 10       | 0.21          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 17       | 0.21          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 19       | 0.21          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 8        | 0.21          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 17       | 0.21          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 1        | 0.2           |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 2        | 0.2           |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 6        | 0.2           |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 1        | 0.2           |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 7        | 0.2           |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 14       | 0.2           |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 3        | 0.2           |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 4        | 0.2           |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 6        | 0.2           |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 8        | 0.2           |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 18       | 0.2           |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 20       | 0.2           |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 15       | 0.2           |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 15       | 0.2           |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 15       | 0.2           |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 20       | 0.2           |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 13       | 0.2           |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 15       | 0.2           |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 3        | 0.2           |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 5        | 0.2           |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 17       | 0.2           |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 10       | 0.2           |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 15       | 0.2           |
| (4,16)  | 1:33:A:LEU:O  | 1:37:A:CYS:N  | 6        | 0.2           |
| (4,16)  | 1:33:A:LEU:O  | 1:37:A:CYS:N  | 17       | 0.2           |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 11       | 0.2           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,11)  | 1:38:A:LEU:O  | 1:42:A:GLY:N  | 5        | 0.2           |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 6        | 0.2           |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 15       | 0.2           |
| (4,4)   | 1:12:A:VAL:O  | 1:16:A:SER:N  | 16       | 0.2           |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 2        | 0.2           |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 9        | 0.2           |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 11       | 0.2           |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 13       | 0.2           |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 14       | 0.2           |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 19       | 0.2           |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 6        | 0.2           |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 19       | 0.2           |
| (1,709) | 1:49:A:ASP:H  | 1:87:A:SER:CB | 12       | 0.2           |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 2        | 0.2           |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 4        | 0.2           |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 6        | 0.2           |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 8        | 0.2           |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 9        | 0.2           |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 10       | 0.2           |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 11       | 0.2           |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 13       | 0.2           |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 15       | 0.2           |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 17       | 0.2           |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 18       | 0.2           |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 14       | 0.2           |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 6        | 0.2           |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 7        | 0.19          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 9        | 0.19          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 10       | 0.19          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 5        | 0.19          |
| (4,32)  | 1:54:A:LYS:O  | 1:58:A:PHE:N  | 5        | 0.19          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 6        | 0.19          |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 9        | 0.19          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 16       | 0.19          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 20       | 0.19          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 1        | 0.19          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 2        | 0.19          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 9        | 0.19          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 18       | 0.19          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 11       | 0.19          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 20       | 0.19          |
| (4,16)  | 1:33:A:LEU:O  | 1:37:A:CYS:N  | 5        | 0.19          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 20       | 0.19          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 15       | 0.19          |
| (4,11)  | 1:38:A:LEU:O  | 1:42:A:GLY:N  | 7        | 0.19          |
| (4,10)  | 1:39:A:ALA:O  | 1:43:A:ALA:N  | 1        | 0.19          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 12       | 0.19          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 1        | 0.19          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 16       | 0.19          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 17       | 0.19          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 1        | 0.19          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 4        | 0.19          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 6        | 0.19          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 7        | 0.19          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 10       | 0.19          |
| (3,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 14       | 0.19          |
| (1,797) | 1:74:A:SER:CB | 1:90:A:MET:H  | 2        | 0.19          |
| (1,783) | 1:67:A:MET:H  | 1:74:A:SER:CB | 20       | 0.19          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 11       | 0.19          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 8        | 0.19          |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 12       | 0.19          |
| (1,634) | 1:37:A:CYS:CB | 1:96:A:LEU:H  | 20       | 0.19          |
| (1,609) | 1:37:A:CYS:CB | 1:63:A:LEU:H  | 16       | 0.19          |
| (1,567) | 1:30:A:ILE:H  | 1:56:A:SER:CB | 5        | 0.19          |
| (1,565) | 1:29:A:LEU:H  | 1:99:A:LEU:CB | 6        | 0.19          |
| (1,514) | 1:20:A:TYR:CB | 1:92:A:LEU:H  | 4        | 0.19          |
| (1,357) | 1:5:A:GLY:H   | 1:20:A:TYR:CB | 16       | 0.19          |
| (1,133) | 1:37:A:CYS:CB | 1:55:A:VAL:H  | 12       | 0.19          |
| (4,87)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 8        | 0.18          |
| (4,44)  | 1:80:A:ALA:O  | 1:84:A:ALA:N  | 12       | 0.18          |
| (4,40)  | 1:84:A:ALA:O  | 1:88:A:LEU:N  | 19       | 0.18          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 15       | 0.18          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 1        | 0.18          |
| (4,29)  | 1:57:A:LEU:O  | 1:61:A:PHE:N  | 4        | 0.18          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 11       | 0.18          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 18       | 0.18          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 13       | 0.18          |
| (4,23)  | 1:63:A:LEU:O  | 1:67:A:MET:N  | 11       | 0.18          |
| (4,21)  | 1:28:A:SER:O  | 1:32:A:GLY:N  | 6        | 0.18          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 2        | 0.18          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 9        | 0.18          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 11       | 0.18          |
| (4,16)  | 1:33:A:LEU:O  | 1:37:A:CYS:N  | 14       | 0.18          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 3        | 0.18          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 9        | 0.18          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 5        | 0.18          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 17       | 0.18          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 10       | 0.18          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 3        | 0.18          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 12       | 0.18          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 13       | 0.18          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 14       | 0.18          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 16       | 0.18          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 17       | 0.18          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 20       | 0.18          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 13       | 0.18          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 4        | 0.18          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 18       | 0.17          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 3        | 0.17          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 9        | 0.17          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 10       | 0.17          |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 11       | 0.17          |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 19       | 0.17          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 2        | 0.17          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 3        | 0.17          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 10       | 0.17          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 6        | 0.17          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 14       | 0.17          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 8        | 0.17          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 20       | 0.17          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 3        | 0.17          |
| (4,3)   | 1:13:A:THR:O  | 1:17:A:ILE:N  | 3        | 0.17          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 8        | 0.17          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 15       | 0.17          |
| (3,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 3        | 0.17          |
| (3,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 4        | 0.17          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 5        | 0.17          |
| (1,797) | 1:74:A:SER:CB | 1:90:A:MET:H  | 9        | 0.17          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 19       | 0.17          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 4        | 0.17          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 3        | 0.17          |
| (1,591) | 1:36:A:GLY:H  | 1:74:A:SER:CB | 6        | 0.17          |
| (1,512) | 1:20:A:TYR:CB | 1:90:A:MET:H  | 17       | 0.17          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 9        | 0.17          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 7        | 0.16          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 9        | 0.16          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 4        | 0.16          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 8        | 0.16          |
| (4,36)  | 1:88:A:LEU:O  | 1:92:A:LEU:N  | 18       | 0.16          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 4        | 0.16          |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 18       | 0.16          |
| (4,24)  | 1:62:A:PHE:O  | 1:66:A:ILE:N  | 8        | 0.16          |
| (4,24)  | 1:62:A:PHE:O  | 1:66:A:ILE:N  | 13       | 0.16          |
| (4,23)  | 1:63:A:LEU:O  | 1:67:A:MET:N  | 8        | 0.16          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 4        | 0.16          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 6        | 0.16          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 19       | 0.16          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 6        | 0.16          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 14       | 0.16          |
| (4,10)  | 1:39:A:ALA:O  | 1:43:A:ALA:N  | 10       | 0.16          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 20       | 0.16          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 5        | 0.16          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 10       | 0.16          |
| (4,3)   | 1:13:A:THR:O  | 1:17:A:ILE:N  | 20       | 0.16          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 8        | 0.16          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 18       | 0.16          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 10       | 0.16          |
| (1,690) | 1:47:A:SER:CB | 1:86:A:LEU:H  | 11       | 0.16          |
| (1,674) | 1:47:A:SER:CB | 1:66:A:ILE:H  | 16       | 0.16          |
| (1,528) | 1:22:A:ARG:H  | 1:37:A:CYS:CB | 10       | 0.16          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 9        | 0.16          |
| (1,514) | 1:20:A:TYR:CB | 1:92:A:LEU:H  | 17       | 0.16          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 7        | 0.16          |
| (1,79)  | 1:26:A:VAL:H  | 1:87:A:SER:CB | 20       | 0.16          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 12       | 0.15          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 14       | 0.15          |
| (4,34)  | 1:90:A:MET:O  | 1:94:A:LEU:N  | 6        | 0.15          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 8        | 0.15          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 3        | 0.15          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 9        | 0.15          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 11       | 0.15          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 18       | 0.15          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 3        | 0.15          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 7        | 0.15          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 12       | 0.15          |
| (4,4)   | 1:12:A:VAL:O  | 1:16:A:SER:N  | 10       | 0.15          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 5        | 0.15          |
| (3,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 16       | 0.15          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 5        | 0.15          |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 17       | 0.15          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 19       | 0.15          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 5        | 0.15          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 11       | 0.15          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 18       | 0.15          |
| (1,412) | 1:13:A:THR:H  | 1:37:A:CYS:CB | 14       | 0.15          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 17       | 0.14          |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 12       | 0.14          |
| (4,35)  | 1:89:A:MET:O  | 1:93:A:ARG:N  | 14       | 0.14          |
| (4,34)  | 1:90:A:MET:O  | 1:94:A:LEU:N  | 20       | 0.14          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 20       | 0.14          |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 16       | 0.14          |
| (4,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:N  | 10       | 0.14          |
| (4,13)  | 1:36:A:GLY:O  | 1:40:A:GLY:N  | 1        | 0.14          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 2        | 0.14          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 4        | 0.14          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 16       | 0.14          |
| (4,7)   | 1:9:A:ALA:O   | 1:13:A:THR:N  | 9        | 0.14          |
| (4,3)   | 1:13:A:THR:O  | 1:17:A:ILE:N  | 2        | 0.14          |
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 2        | 0.14          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 16       | 0.14          |
| (1,710) | 1:49:A:ASP:H  | 1:99:A:LEU:CB | 14       | 0.14          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 4        | 0.14          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 18       | 0.14          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 9        | 0.14          |
| (4,47)  | 1:14:A:PHE:O  | 1:18:A:PHE:H  | 16       | 0.13          |
| (4,39)  | 1:85:A:GLY:O  | 1:89:A:MET:N  | 20       | 0.13          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 12       | 0.13          |
| (4,26)  | 1:60:A:ALA:O  | 1:64:A:ALA:N  | 1        | 0.13          |
| (4,23)  | 1:63:A:LEU:O  | 1:67:A:MET:N  | 7        | 0.13          |
| (4,23)  | 1:63:A:LEU:O  | 1:67:A:MET:N  | 10       | 0.13          |
| (4,23)  | 1:63:A:LEU:O  | 1:67:A:MET:N  | 13       | 0.13          |
| (4,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:N  | 1        | 0.13          |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 18       | 0.13          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 19       | 0.13          |
| (4,16)  | 1:33:A:LEU:O  | 1:37:A:CYS:N  | 13       | 0.13          |
| (4,14)  | 1:35:A:VAL:O  | 1:39:A:ALA:N  | 8        | 0.13          |
| (4,10)  | 1:39:A:ALA:O  | 1:43:A:ALA:N  | 4        | 0.13          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 10       | 0.13          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 11       | 0.13          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 17       | 0.13          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (4,2)   | 1:14:A:PHE:O  | 1:18:A:PHE:N  | 17       | 0.13          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 7        | 0.13          |
| (1,751) | 1:56:A:SER:CB | 1:97:A:LEU:H  | 11       | 0.13          |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 9        | 0.13          |
| (1,694) | 1:47:A:SER:CB | 1:90:A:MET:H  | 8        | 0.13          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 4        | 0.13          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 13       | 0.13          |
| (1,645) | 1:41:A:TYR:H  | 1:56:A:SER:CB | 17       | 0.13          |
| (1,567) | 1:30:A:ILE:H  | 1:56:A:SER:CB | 16       | 0.13          |
| (1,553) | 1:26:A:VAL:H  | 1:74:A:SER:CB | 12       | 0.13          |
| (1,552) | 1:26:A:VAL:H  | 1:56:A:SER:CB | 2        | 0.13          |
| (1,550) | 1:26:A:VAL:H  | 1:37:A:CYS:CB | 1        | 0.13          |
| (1,533) | 1:23:A:ARG:H  | 1:37:A:CYS:CB | 15       | 0.13          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 16       | 0.13          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 6        | 0.13          |
| (1,503) | 1:20:A:TYR:CB | 1:82:A:LEU:H  | 14       | 0.13          |
| (1,226) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 6        | 0.13          |
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 2        | 0.13          |
| (4,87)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 6        | 0.12          |
| (4,42)  | 1:82:A:LEU:O  | 1:86:A:LEU:N  | 14       | 0.12          |
| (4,34)  | 1:90:A:MET:O  | 1:94:A:LEU:N  | 3        | 0.12          |
| (4,34)  | 1:90:A:MET:O  | 1:94:A:LEU:N  | 10       | 0.12          |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 13       | 0.12          |
| (4,20)  | 1:29:A:LEU:O  | 1:33:A:LEU:N  | 4        | 0.12          |
| (4,16)  | 1:33:A:LEU:O  | 1:37:A:CYS:N  | 2        | 0.12          |
| (4,16)  | 1:33:A:LEU:O  | 1:37:A:CYS:N  | 8        | 0.12          |
| (4,11)  | 1:38:A:LEU:O  | 1:42:A:GLY:N  | 9        | 0.12          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 13       | 0.12          |
| (4,6)   | 1:10:A:ALA:O  | 1:14:A:PHE:N  | 14       | 0.12          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 11       | 0.12          |
| (1,797) | 1:74:A:SER:CB | 1:90:A:MET:H  | 12       | 0.12          |
| (1,786) | 1:68:A:GLY:H  | 1:74:A:SER:CB | 20       | 0.12          |
| (1,748) | 1:56:A:SER:CB | 1:94:A:LEU:H  | 7        | 0.12          |
| (1,691) | 1:47:A:SER:CB | 1:87:A:SER:H  | 2        | 0.12          |
| (1,635) | 1:37:A:CYS:CB | 1:97:A:LEU:H  | 20       | 0.12          |
| (1,563) | 1:29:A:LEU:H  | 1:74:A:SER:CB | 11       | 0.12          |
| (1,523) | 1:21:A:LYS:H  | 1:37:A:CYS:CB | 13       | 0.12          |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 1        | 0.12          |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 2        | 0.12          |
| (1,421) | 1:14:A:PHE:H  | 1:87:A:SER:CB | 3        | 0.12          |
| (1,397) | 1:10:A:ALA:H  | 1:87:A:SER:CB | 13       | 0.12          |
| (1,226) | 1:50:A:LYS:H  | 1:99:A:LEU:CB | 1        | 0.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,192) | 1:46:A:VAL:H  | 1:56:A:SER:CB | 17       | 0.12          |
| (4,43)  | 1:81:A:GLY:O  | 1:85:A:GLY:N  | 12       | 0.11          |
| (4,38)  | 1:86:A:LEU:O  | 1:90:A:MET:N  | 16       | 0.11          |
| (4,34)  | 1:90:A:MET:O  | 1:94:A:LEU:N  | 12       | 0.11          |
| (4,34)  | 1:90:A:MET:O  | 1:94:A:LEU:N  | 14       | 0.11          |
| (4,34)  | 1:90:A:MET:O  | 1:94:A:LEU:N  | 16       | 0.11          |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 12       | 0.11          |
| (4,27)  | 1:59:A:THR:O  | 1:63:A:LEU:N  | 14       | 0.11          |
| (4,20)  | 1:29:A:LEU:O  | 1:33:A:LEU:N  | 7        | 0.11          |
| (4,20)  | 1:29:A:LEU:O  | 1:33:A:LEU:N  | 14       | 0.11          |
| (4,17)  | 1:32:A:GLY:O  | 1:36:A:GLY:N  | 14       | 0.11          |
| (4,15)  | 1:34:A:PHE:O  | 1:38:A:LEU:N  | 17       | 0.11          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 1        | 0.11          |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 13       | 0.11          |
| (4,8)   | 1:8:A:TYR:O   | 1:12:A:VAL:N  | 18       | 0.11          |
| (4,5)   | 1:11:A:LEU:O  | 1:15:A:GLY:N  | 20       | 0.11          |
| (4,4)   | 1:12:A:VAL:O  | 1:16:A:SER:N  | 6        | 0.11          |
| (4,3)   | 1:13:A:THR:O  | 1:17:A:ILE:N  | 8        | 0.11          |
| (4,1)   | 1:15:A:GLY:O  | 1:19:A:GLY:N  | 19       | 0.11          |
| (3,22)  | 1:64:A:ALA:O  | 1:68:A:GLY:H  | 20       | 0.11          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 1        | 0.11          |
| (1,819) | 1:87:A:SER:CB | 1:99:A:LEU:H  | 18       | 0.11          |
| (1,797) | 1:74:A:SER:CB | 1:90:A:MET:H  | 14       | 0.11          |
| (1,718) | 1:52:A:ASP:H  | 1:99:A:LEU:CB | 3        | 0.11          |
| (1,712) | 1:50:A:LYS:H  | 1:87:A:SER:CB | 2        | 0.11          |
| (1,657) | 1:44:A:TYR:H  | 1:87:A:SER:CB | 18       | 0.11          |
| (1,546) | 1:25:A:GLY:H  | 1:56:A:SER:CB | 18       | 0.11          |
| (1,516) | 1:20:A:TYR:CB | 1:94:A:LEU:H  | 15       | 0.11          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 11       | 0.11          |
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 20       | 0.11          |
| (4,43)  | 1:81:A:GLY:O  | 1:85:A:GLY:N  | 14       | 0.1           |
| (4,37)  | 1:87:A:SER:O  | 1:91:A:ILE:N  | 20       | 0.1           |
| (4,34)  | 1:90:A:MET:O  | 1:94:A:LEU:N  | 9        | 0.1           |
| (4,30)  | 1:56:A:SER:O  | 1:60:A:ALA:N  | 18       | 0.1           |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 1        | 0.1           |
| (4,25)  | 1:61:A:PHE:O  | 1:65:A:THR:N  | 9        | 0.1           |
| (4,20)  | 1:29:A:LEU:O  | 1:33:A:LEU:N  | 5        | 0.1           |
| (4,20)  | 1:29:A:LEU:O  | 1:33:A:LEU:N  | 15       | 0.1           |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 12       | 0.1           |
| (4,19)  | 1:30:A:ILE:O  | 1:34:A:PHE:N  | 13       | 0.1           |
| (4,11)  | 1:38:A:LEU:O  | 1:42:A:GLY:N  | 18       | 0.1           |
| (4,9)   | 1:40:A:GLY:O  | 1:44:A:TYR:N  | 5        | 0.1           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (1,515) | 1:20:A:TYR:CB | 1:93:A:ARG:H  | 15       | 0.1           |
| (1,506) | 1:20:A:TYR:CB | 1:85:A:GLY:H  | 4        | 0.1           |
| (1,435) | 1:17:A:ILE:H  | 1:37:A:CYS:CB | 19       | 0.1           |
| (1,343) | 1:3:A:LEU:H   | 1:20:A:TYR:CB | 5        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found