# Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 06:41 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 2PXG |
| BMRB ID | : | 6797 |
| Title | : | NMR Solution Structure of OmlA |
| Authors | : | Vanini, M.M.T.; Pertinhez, T.A.; Sforca, M.L.; Spisni, A.; Benedetti, C.E. |
| Deposited on | : | 2007-05-14 |

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

We welcome your comments at *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 (i) 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 (i)) were used in the production of this report:

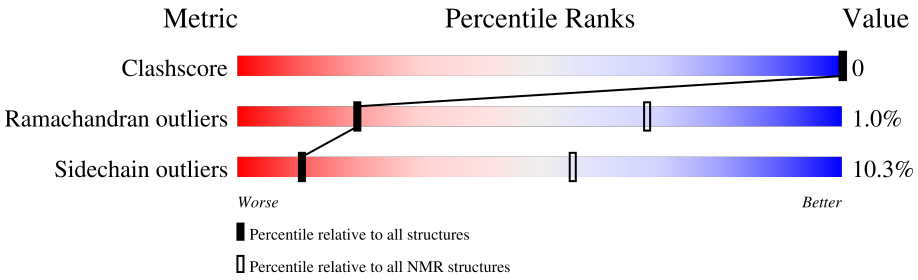
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| BMRB Restraints Analysis | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.33 |

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 91%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|---|---|---|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

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 >=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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 118 | 49% . . 44% |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| **Well-defined core** | **Residue range (total)** | **Backbone RMSD (Å)** | **Medoid model** |
| 1 | A:18-A:56, A:70-A:88 (58) | 1.14 | 15 |
| 2 | A:105-A:112 (8) | 1.86 | 8 |

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

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

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

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

# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1915 atoms, of which 954 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Outer membrane protein.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 1 | A | 118 | 1915 | 604 | 954 | 178 | 178 | 1 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | MET | - | initiating methionine | UNP Q8PMB6 |
| A | 4 | SER | CYS | engineered mutation | UNP Q8PMB6 |

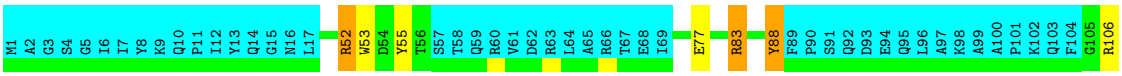
# 4 Residue-property plots

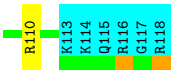
## 4.1 Average score per residue in the NMR ensemble

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: Outer membrane protein

Chain A:

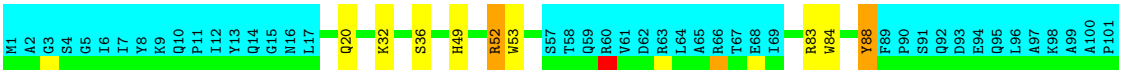

## 4.2 Scores per residue for each member of the ensemble

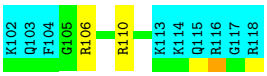
Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: Outer membrane protein

Chain A:

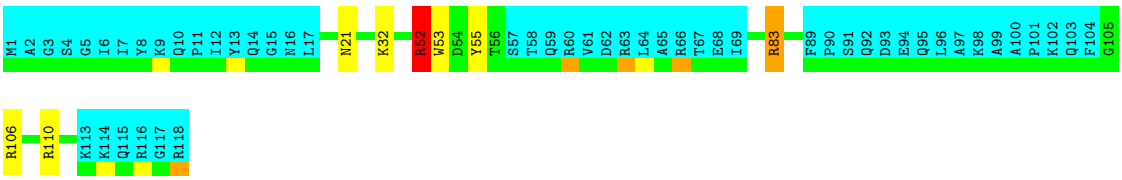




### 4.2.2 Score per residue for model 2

• Molecule 1: Outer membrane protein

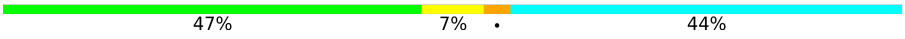
Chain A:

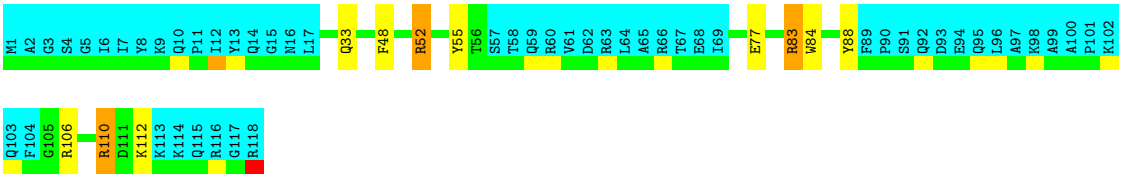



### 4.2.3 Score per residue for model 3

• Molecule 1: Outer membrane protein

Chain A:

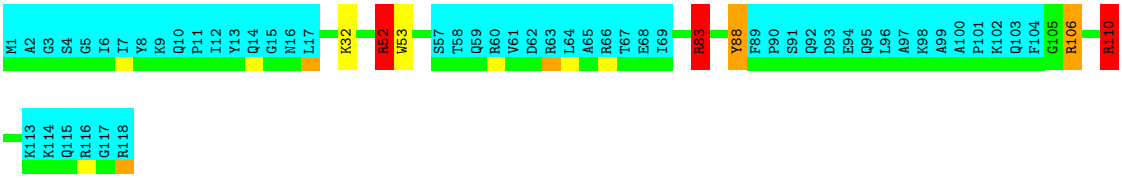



### 4.2.4 Score per residue for model 4

• Molecule 1: Outer membrane protein

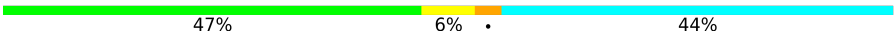
Chain A:

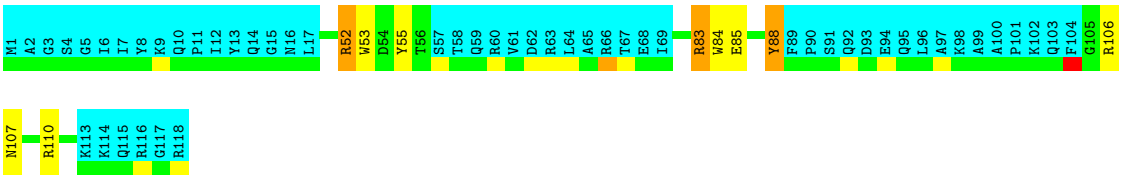




### 4.2.5 Score per residue for model 5

• Molecule 1: Outer membrane protein

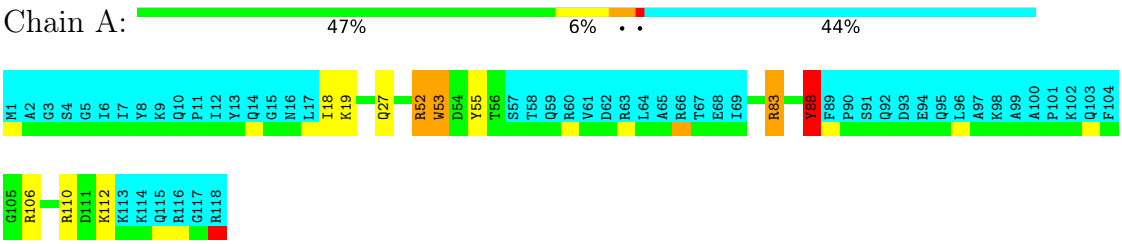
Chain A:



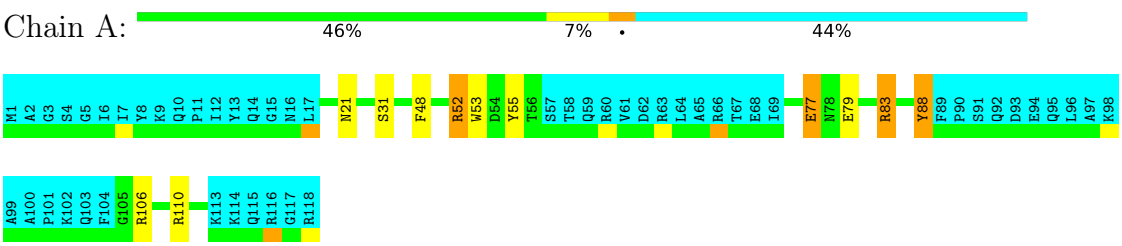

### 4.2.6 Score per residue for model 6

• Molecule 1: Outer membrane protein



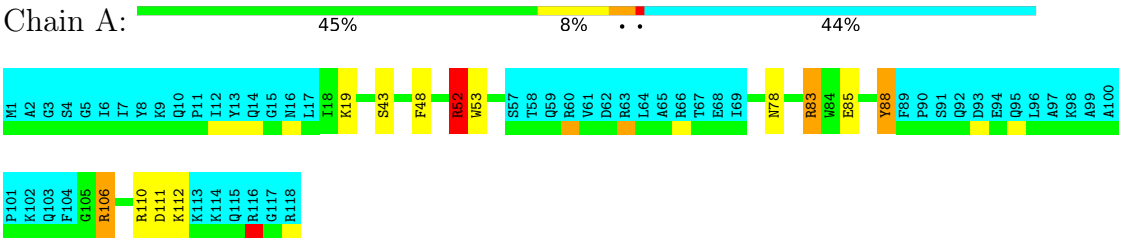

### 4.2.7 Score per residue for model 7

• Molecule 1: Outer membrane protein



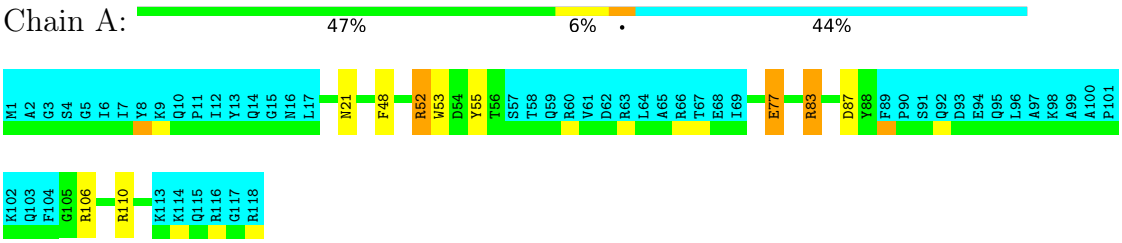

### 4.2.8 Score per residue for model 8

• Molecule 1: Outer membrane protein




### 4.2.9 Score per residue for model 9

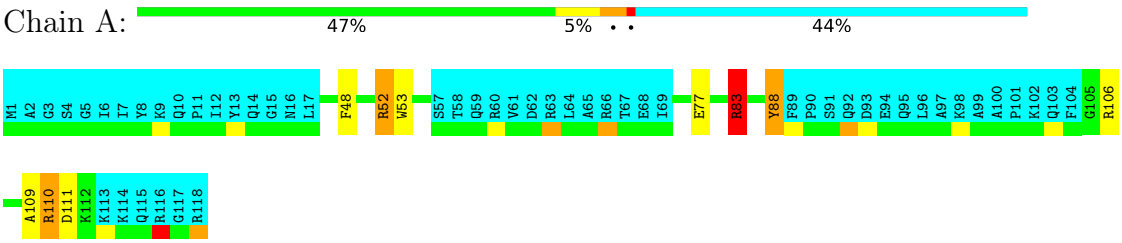
• Molecule 1: Outer membrane protein



### 4.2.10 Score per residue for model 10

• Molecule 1: Outer membrane protein

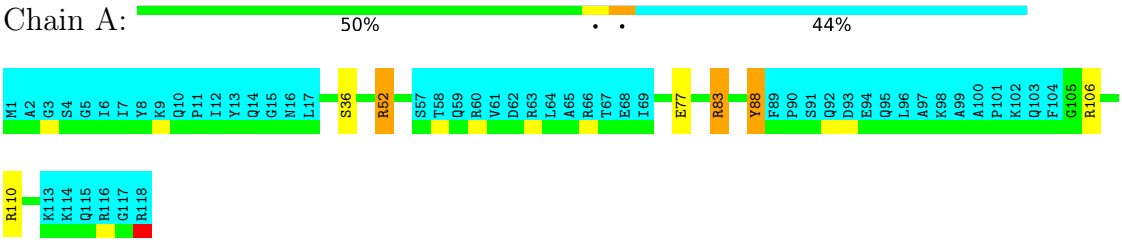
Chain A:




### 4.2.11 Score per residue for model 11

• Molecule 1: Outer membrane protein

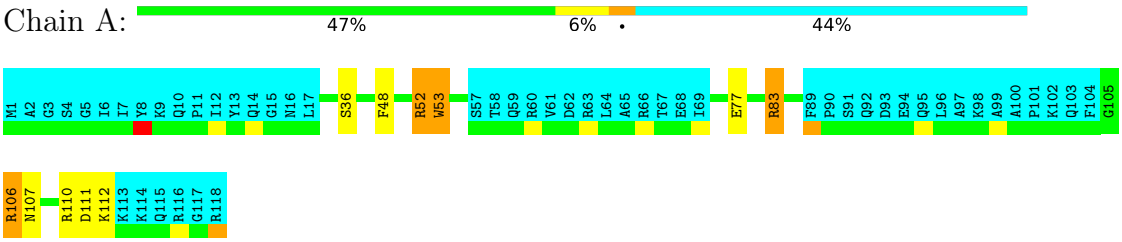
Chain A:




### 4.2.12 Score per residue for model 12

• Molecule 1: Outer membrane protein

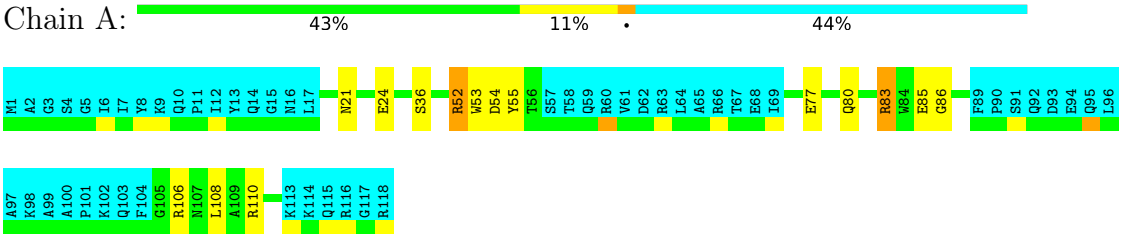
Chain A:




### 4.2.13 Score per residue for model 13

• Molecule 1: Outer membrane protein

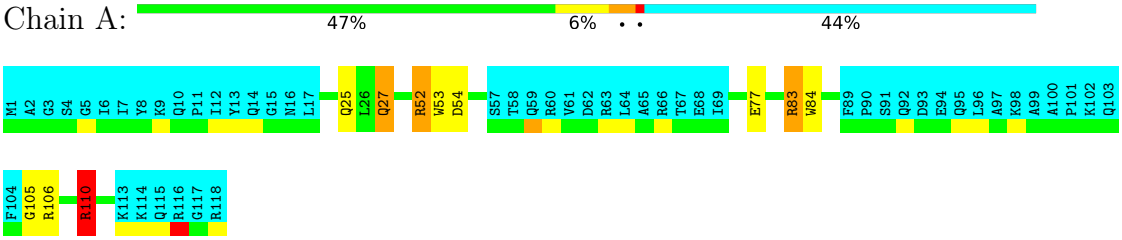
Chain A:



### 4.2.14 Score per residue for model 14

• Molecule 1: Outer membrane protein

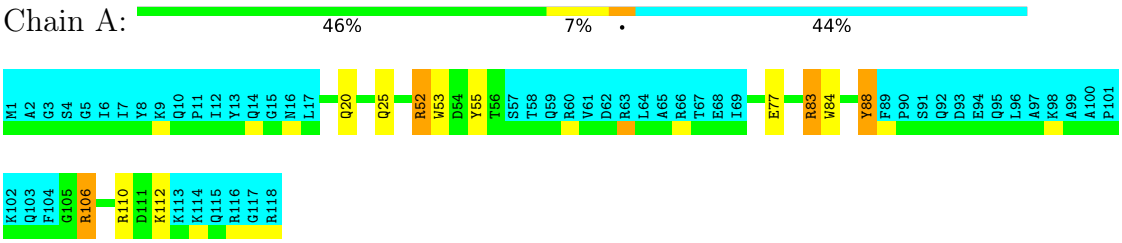
Chain A:




### 4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: Outer membrane protein

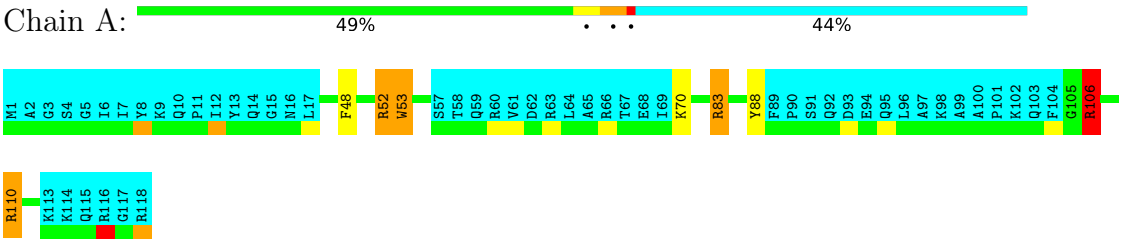
Chain A:




### 4.2.16 Score per residue for model 16

• Molecule 1: Outer membrane protein

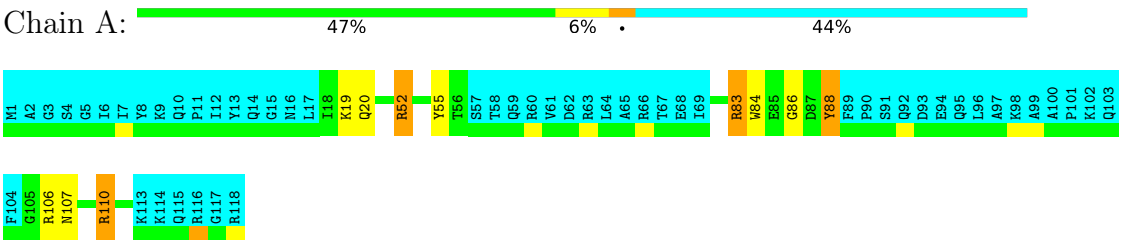
Chain A:




### 4.2.17 Score per residue for model 17

• Molecule 1: Outer membrane protein

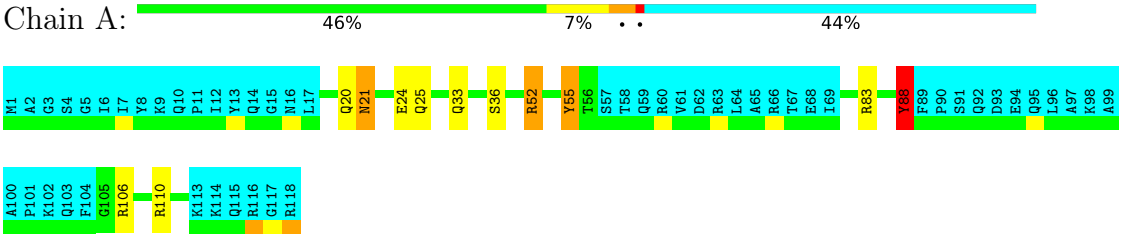
Chain A:



### 4.2.18 Score per residue for model 18

• Molecule 1: Outer membrane protein

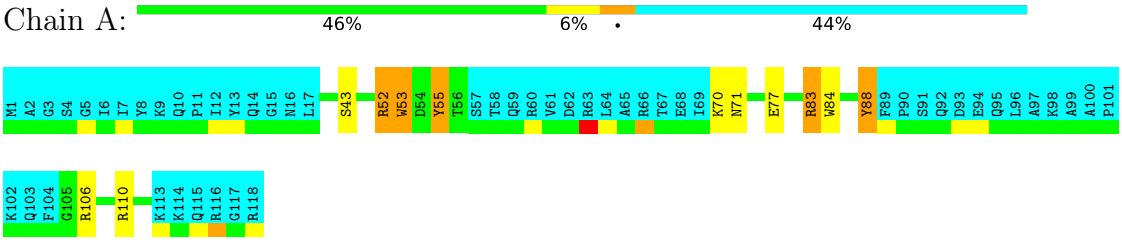
Chain A:




### 4.2.19 Score per residue for model 19

• Molecule 1: Outer membrane protein

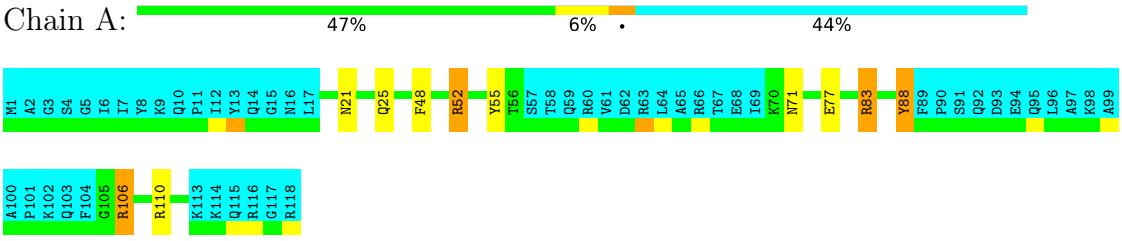
Chain A:




### 4.2.20 Score per residue for model 20

• Molecule 1: Outer membrane protein

Chain A:



# 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

| Software name | Classification | Version |
|---|---|---|
| DYANA | structure solution | |
| Discover | 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 | 1512 |
| Number of shifts mapped to atoms | 1512 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 91% |

# 6 Model quality

## 6.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 1.07±0.01 | 0±0/558 ( 0.0± 0.0%) | 1.49±0.04 | 9±2/757 ( 1.1± 0.3%) |
| All | All | 1.07 | 0/11160 ( 0.0%) | 1.49 | 172/15140 ( 1.1%) |

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

| Mol | Chain | Chirality | Planarity |
|---|---|---|---|
| 1 | A | 0.0±0.0 | 2.2±1.2 |
| All | All | 0 | 44 |

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 88 | TYR | CB-CG-CD2 | -10.22 | 114.87 | 121.00 | 6 | 11 |
| 1 | A | 110 | ARG | NE-CZ-NH1 | 9.90 | 125.25 | 120.30 | 6 | 20 |
| 1 | A | 52 | ARG | NE-CZ-NH1 | 9.85 | 125.22 | 120.30 | 9 | 20 |
| 1 | A | 106 | ARG | NE-CZ-NH1 | 9.64 | 125.12 | 120.30 | 13 | 20 |
| 1 | A | 83 | ARG | NE-CZ-NH1 | 9.29 | 124.95 | 120.30 | 14 | 20 |
| 1 | A | 88 | TYR | CB-CG-CD1 | 8.92 | 126.35 | 121.00 | 18 | 10 |
| 1 | A | 55 | TYR | CB-CG-CD2 | -8.87 | 115.68 | 121.00 | 19 | 5 |
| 1 | A | 52 | ARG | NE-CZ-NH2 | -8.85 | 115.88 | 120.30 | 16 | 13 |
| 1 | A | 55 | TYR | CB-CG-CD1 | 8.25 | 125.95 | 121.00 | 19 | 4 |
| 1 | A | 106 | ARG | NE-CZ-NH2 | -7.46 | 116.57 | 120.30 | 5 | 3 |
| 1 | A | 110 | ARG | NE-CZ-NH2 | -6.77 | 116.92 | 120.30 | 15 | 7 |
| 1 | A | 53 | TRP | CA-CB-CG | 6.38 | 125.82 | 113.70 | 16 | 5 |
| 1 | A | 88 | TYR | CA-CB-CG | 6.37 | 125.51 | 113.40 | 1 | 3 |
| 1 | A | 55 | TYR | CA-CB-CG | 6.12 | 125.03 | 113.40 | 18 | 1 |
| 1 | A | 83 | ARG | NE-CZ-NH2 | -6.00 | 117.30 | 120.30 | 2 | 8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 53 | TRP | CD1-NE1-CE2 | -5.60 | 103.96 | 109.00 | 19 | 15 |
| 1 | A | 88 | TYR | N-CA-C | 5.47 | 125.77 | 111.00 | 18 | 1 |
| 1 | A | 84 | TRP | CD1-NE1-CE2 | -5.36 | 104.18 | 109.00 | 14 | 6 |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group | Models (Total) |
|---|---|---|---|---|---|
| 1 | A | 55 | TYR | Sidechain | 8 |
| 1 | A | 77 | GLU | Peptide | 8 |
| 1 | A | 52 | ARG | Sidechain | 4 |
| 1 | A | 110 | ARG | Sidechain,Peptide | 3 |
| 1 | A | 88 | TYR | Sidechain | 3 |
| 1 | A | 83 | ARG | Sidechain | 2 |
| 1 | A | 106 | ARG | Peptide,Sidechain | 2 |
| 1 | A | 54 | ASP | Peptide | 2 |
| 1 | A | 86 | GLY | Peptide | 2 |
| 1 | A | 84 | TRP | Peptide | 1 |
| 1 | A | 18 | ILE | Peptide | 1 |
| 1 | A | 112 | LYS | Peptide | 1 |
| 1 | A | 78 | ASN | Peptide | 1 |
| 1 | A | 111 | ASP | Peptide | 1 |
| 1 | A | 87 | ASP | Peptide | 1 |
| 1 | A | 109 | ALA | Peptide | 1 |
| 1 | A | 20 | GLN | Peptide | 1 |
| 1 | A | 19 | LYS | Peptide | 1 |
| 1 | A | 71 | ASN | Peptide | 1 |

## 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 | 544 | 522 | 522 | 0±0 |
| All | All | 10880 | 10440 | 10440 | 1 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:A:31:SER:OG | 1:A:79:GLU:OE2 | 0.40 | 2.34 | 7 | 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 | 66/118 (56%) | 49±2 (74±4%) | 16±2 (25±4%) | 1±1 (1±1%) | 20 | 68 |
| All | All | 1320/2360 (56%) | 979 (74%) | 328 (25%) | 13 (1%) | 20 | 68 |

All 7 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 | 21 | ASN | 5 |
| 1 | A | 43 | SER | 2 |
| 1 | A | 88 | TYR | 2 |
| 1 | A | 107 | ASN | 1 |
| 1 | A | 85 | GLU | 1 |
| 1 | A | 27 | GLN | 1 |
| 1 | A | 105 | GLY | 1 |

### 6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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 | 58/101 (57%) | 52±2 (90±3%) | 6±2 (10±3%) | 11 | 55 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| All | All | 1160/2020 (57%) | 1040 (90%) | 120 (10%) | 11 55 |

All 27 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 | 52 | ARG | 19 |
| 1 | A | 83 | ARG | 18 |
| 1 | A | 88 | TYR | 14 |
| 1 | A | 48 | PHE | 8 |
| 1 | A | 36 | SER | 5 |
| 1 | A | 77 | GLU | 5 |
| 1 | A | 110 | ARG | 5 |
| 1 | A | 106 | ARG | 5 |
| 1 | A | 112 | LYS | 4 |
| 1 | A | 53 | TRP | 4 |
| 1 | A | 25 | GLN | 4 |
| 1 | A | 20 | GLN | 3 |
| 1 | A | 32 | LYS | 3 |
| 1 | A | 33 | GLN | 2 |
| 1 | A | 85 | GLU | 2 |
| 1 | A | 19 | LYS | 2 |
| 1 | A | 27 | GLN | 2 |
| 1 | A | 111 | ASP | 2 |
| 1 | A | 107 | ASN | 2 |
| 1 | A | 21 | ASN | 2 |
| 1 | A | 24 | GLU | 2 |
| 1 | A | 70 | LYS | 2 |
| 1 | A | 49 | HIS | 1 |
| 1 | A | 80 | GLN | 1 |
| 1 | A | 108 | LEU | 1 |
| 1 | A | 55 | TYR | 1 |
| 1 | A | 71 | ASN | 1 |

### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry (i)

There are no ligands in this entry.

## 6.7 Other polymers (i)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% 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 | 1512 |
| Number of shifts mapped to atoms | 1512 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 6 |

### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 118 | 0.51 ± 0.11 | Should be applied |
| $^{13}C_{\beta}$ | 110 | 0.63 ± 0.11 | Should be applied |
| $^{13}C'$ | 111 | -0.42 ± 0.10 | None needed (< 0.5 ppm) |
| $^{15}N$ | 111 | -1.28 ± 0.42 | Should be applied |

### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 849 atoms were assigned a chemical shift out of a possible 928. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 325/328 (99%) | 133/133 (100%) | 129/132 (98%) | 63/63 (100%) |
| Sidechain | 450/511 (88%) | 298/326 (91%) | 137/157 (87%) | 15/28 (54%) |

*Continued on next page...*

*Continued from previous page...*

| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Aromatic | 74/89 (83%) | 38/44 (86%) | 34/42 (81%) | 2/3 (67%) |
| Overall | 849/928 (91%) | 469/503 (93%) | 300/331 (91%) | 80/94 (85%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1512 atoms were assigned a chemical shift out of a possible 1669. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}$H | $^{13}$C | $^{15}$N |
|---|---|---|---|---|
| Backbone | 577/586 (98%) | 237/238 (100%) | 229/236 (97%) | 111/112 (99%) |
| Sidechain | 837/956 (88%) | 556/611 (91%) | 255/289 (88%) | 26/56 (46%) |
| Aromatic | 98/127 (77%) | 50/62 (81%) | 46/62 (74%) | 2/3 (67%) |
| Overall | 1512/1669 (91%) | 843/911 (93%) | 530/587 (90%) | 139/171 (81%) |

### 7.1.4 Statistically unusual chemical shifts (i)

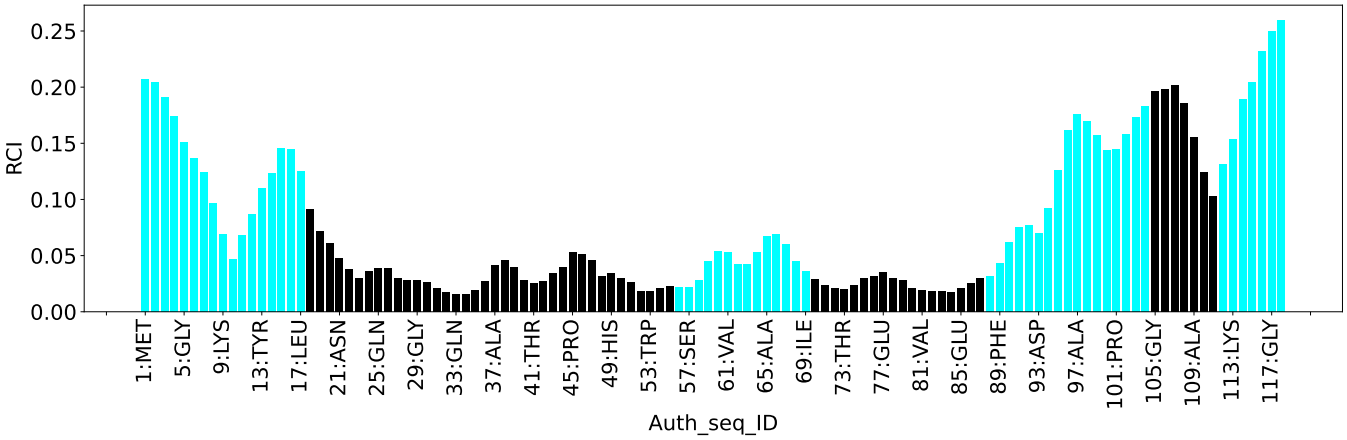
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, *ppm* | Expected range, *ppm* | Z-score |
|---|---|---|---|---|---|---|---|
| 1 | A | 60 | ARG | NE | 124.66 | 76.53 – 92.65 | 24.9 |
| 1 | A | 52 | ARG | NE | 113.74 | 76.53 – 92.65 | 18.1 |
| 1 | A | 110 | ARG | NE | 111.15 | 76.53 – 92.65 | 16.5 |
| 1 | A | 118 | ARG | NE | 111.15 | 76.53 – 92.65 | 16.5 |
| 1 | A | 63 | ARG | NE | 110.76 | 76.53 – 92.65 | 16.2 |
| 1 | A | 83 | ARG | NE | 109.76 | 76.53 – 92.65 | 15.6 |

### 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:


RCI
0.25
0.20
0.15
0.10
0.05
0.00
1:MET
5:GLY
9:LYS
13:TYR
17:LEU
21:ASN
25:GLN
29:GLY
33:GLN
37:ALA
41:THR
45:PRO
49:HIS
53:TRP
57:SER
61:VAL
65:ALA
69:ILE
73:THR
77:GLU
81:VAL
85:GLU
89:PHE
93:ASP
97:ALA
101:PRO
105:GLY
109:ALA
113:LYS
117:GLY
Auth_seq_ID

# 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 | 712 |
| Intra-residue (\|i-j\|=0) | 255 |
| Sequential (\|i-j\|=1) | 271 |
| Medium range (\|i-j\|>1 and \|i-j\|<5) | 78 |
| Long range (\|i-j\|≥5) | 108 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 0 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 6.0 |
| Number of long range restraints per residue[1] | 0.9 |

[1]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) | 37.8 | 0.2 |
| 0.2-0.5 (Medium) | 31.4 | 0.5 |
| >0.5 (Large) | 59.8 | 8.6 |

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

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

# 9 Distance violation analysis (i)

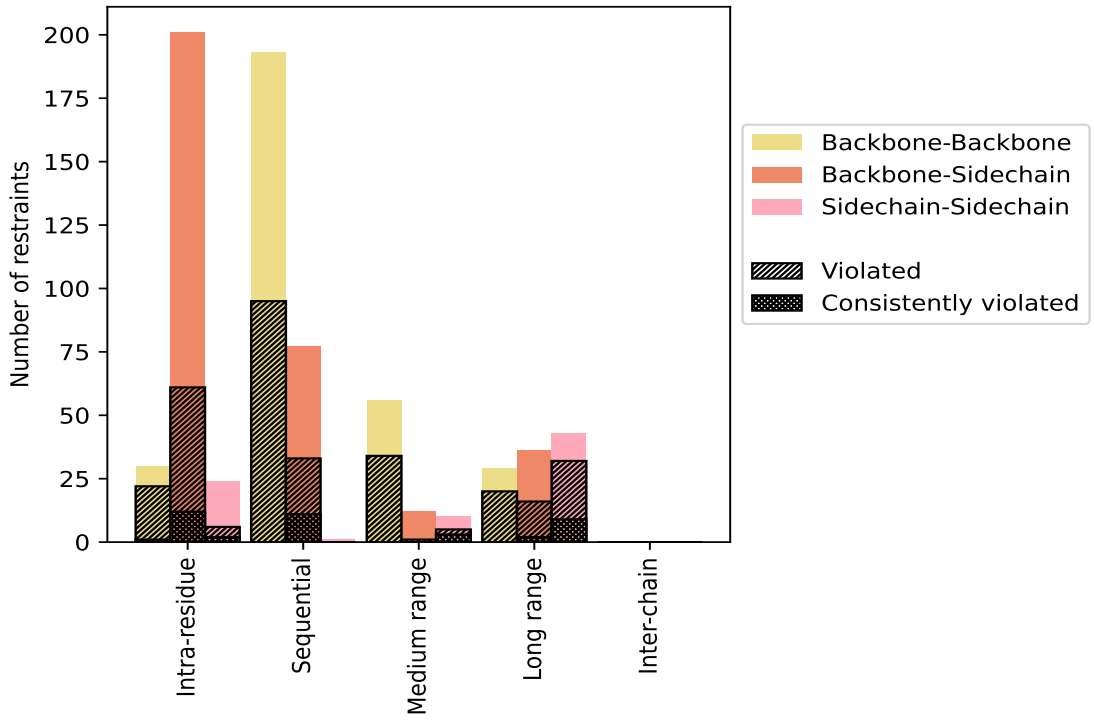
## 9.1 Summary of distance violations (i)

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.

| Restraints type | Count | %[1] | Violated[3] | | | Consistently Violated[4] | | |
|---|---|---|---|---|---|---|---|---|
| | | | Count | %[2] | %[1] | Count | %[2] | %[1] |
| Intra-residue (\|i-j\|=0) | 255 | 35.8 | 89 | 34.9 | 12.5 | 15 | 5.9 | 2.1 |
| Backbone-Backbone | 30 | 4.2 | 22 | 73.3 | 3.1 | 1 | 3.3 | 0.1 |
| Backbone-Sidechain | 201 | 28.2 | 61 | 30.3 | 8.6 | 12 | 6.0 | 1.7 |
| Sidechain-Sidechain | 24 | 3.4 | 6 | 25.0 | 0.8 | 2 | 8.3 | 0.3 |
| Sequential (\|i-j\|=1) | 271 | 38.1 | 128 | 47.2 | 18.0 | 11 | 4.1 | 1.5 |
| Backbone-Backbone | 193 | 27.1 | 95 | 49.2 | 13.3 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 77 | 10.8 | 33 | 42.9 | 4.6 | 11 | 14.3 | 1.5 |
| Sidechain-Sidechain | 1 | 0.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Medium range (\|i-j\|>1 & \|i-j\|<5) | 78 | 11.0 | 40 | 51.3 | 5.6 | 3 | 3.8 | 0.4 |
| Backbone-Backbone | 56 | 7.9 | 34 | 60.7 | 4.8 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 12 | 1.7 | 1 | 8.3 | 0.1 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 10 | 1.4 | 5 | 50.0 | 0.7 | 3 | 30.0 | 0.4 |
| Long range (\|i-j\|≥5) | 108 | 15.2 | 68 | 63.0 | 9.6 | 11 | 10.2 | 1.5 |
| Backbone-Backbone | 29 | 4.1 | 20 | 69.0 | 2.8 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 36 | 5.1 | 16 | 44.4 | 2.2 | 2 | 5.6 | 0.3 |
| Sidechain-Sidechain | 43 | 6.0 | 32 | 74.4 | 4.5 | 9 | 20.9 | 1.3 |
| 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 | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 712 | 100.0 | 325 | 45.6 | 45.6 | 40 | 5.6 | 5.6 |
| Backbone-Backbone | 308 | 43.3 | 171 | 55.5 | 24.0 | 1 | 0.3 | 0.1 |
| Backbone-Sidechain | 326 | 45.8 | 111 | 34.0 | 15.6 | 25 | 7.7 | 3.5 |
| Sidechain-Sidechain | 78 | 11.0 | 43 | 55.1 | 6.0 | 14 | 17.9 | 2.0 |

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

### 9.1.1 Bar chart : Distribution of distance restraints and violations




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

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[6] (Å) | Median (Å) |
|---|---|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | | | |
| 1 | 48 | 40 | 15 | 40 | 0 | 143 | 0.59 | 3.51 | 0.6 | 0.33 |
| 2 | 42 | 32 | 8 | 32 | 0 | 114 | 0.77 | 7.61 | 0.94 | 0.54 |
| 3 | 36 | 39 | 11 | 32 | 0 | 118 | 0.82 | 6.41 | 1.0 | 0.48 |
| 4 | 38 | 32 | 13 | 39 | 0 | 122 | 0.81 | 8.16 | 1.05 | 0.52 |
| 5 | 39 | 38 | 14 | 37 | 0 | 128 | 0.7 | 4.11 | 0.76 | 0.44 |
| 6 | 39 | 41 | 15 | 34 | 0 | 129 | 0.75 | 6.45 | 0.9 | 0.46 |
| 7 | 41 | 36 | 12 | 35 | 0 | 124 | 0.74 | 7.79 | 0.99 | 0.45 |
| 8 | 35 | 40 | 10 | 39 | 0 | 124 | 0.69 | 7.03 | 0.87 | 0.44 |
| 9 | 45 | 34 | 9 | 35 | 0 | 123 | 0.69 | 7.7 | 0.87 | 0.49 |
| 10 | 39 | 42 | 11 | 42 | 0 | 134 | 0.78 | 7.24 | 0.97 | 0.48 |
| 11 | 43 | 35 | 13 | 35 | 0 | 126 | 0.79 | 6.57 | 0.95 | 0.5 |

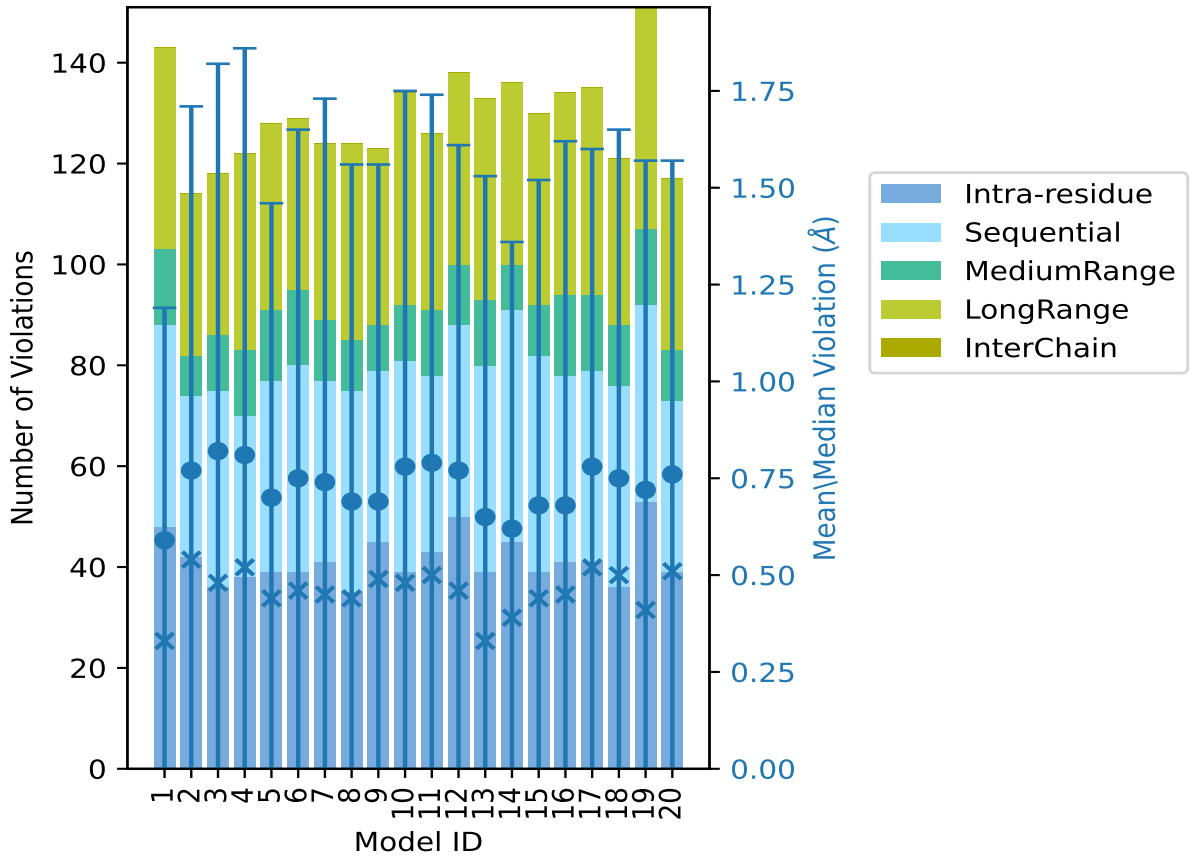
*Continued on next page...*

*Continued from previous page...*

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD[6] (Å) | Median (Å) |
|---|---|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | | | |
| 12 | 50 | 38 | 12 | 38 | 0 | 138 | 0.77 | 5.54 | 0.84 | 0.46 |
| 13 | 39 | 41 | 13 | 40 | 0 | 133 | 0.65 | 7.67 | 0.88 | 0.33 |
| 14 | 45 | 46 | 9 | 36 | 0 | 136 | 0.62 | 5.57 | 0.74 | 0.39 |
| 15 | 39 | 43 | 10 | 38 | 0 | 130 | 0.68 | 5.75 | 0.84 | 0.44 |
| 16 | 41 | 37 | 16 | 40 | 0 | 134 | 0.68 | 8.6 | 0.94 | 0.45 |
| 17 | 41 | 38 | 15 | 41 | 0 | 135 | 0.78 | 4.2 | 0.82 | 0.52 |
| 18 | 36 | 40 | 12 | 33 | 0 | 121 | 0.75 | 6.74 | 0.9 | 0.5 |
| 19 | 53 | 39 | 15 | 44 | 0 | 151 | 0.72 | 5.2 | 0.85 | 0.41 |
| 20 | 39 | 34 | 10 | 34 | 0 | 117 | 0.76 | 4.05 | 0.81 | 0.51 |

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]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

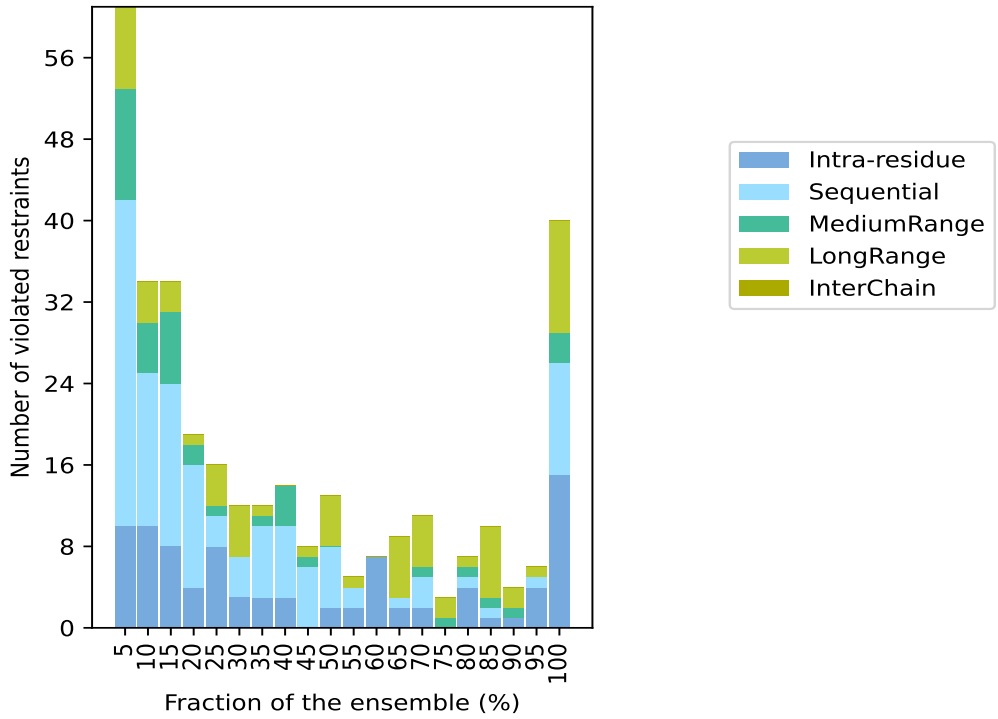
## 9.3 Distance violation statistics for the ensemble (i)

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, 387(IR:166, SQ:143, MR:38, LR:40, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|---|---|---|---|---|---|---|---|
| IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | Count[6] | % |
| 10 | 32 | 11 | 8 | 0 | 61 | 1 | 5.0 |
| 10 | 15 | 5 | 4 | 0 | 34 | 2 | 10.0 |
| 8 | 16 | 7 | 3 | 0 | 34 | 3 | 15.0 |
| 4 | 12 | 2 | 1 | 0 | 19 | 4 | 20.0 |
| 8 | 3 | 1 | 4 | 0 | 16 | 5 | 25.0 |
| 3 | 4 | 0 | 5 | 0 | 12 | 6 | 30.0 |
| 3 | 7 | 1 | 1 | 0 | 12 | 7 | 35.0 |
| 3 | 7 | 4 | 0 | 0 | 14 | 8 | 40.0 |
| 0 | 6 | 1 | 1 | 0 | 8 | 9 | 45.0 |
| 2 | 6 | 0 | 5 | 0 | 13 | 10 | 50.0 |
| 2 | 2 | 0 | 1 | 0 | 5 | 11 | 55.0 |
| 7 | 0 | 0 | 0 | 0 | 7 | 12 | 60.0 |
| 2 | 1 | 0 | 6 | 0 | 9 | 13 | 65.0 |
| 2 | 3 | 1 | 5 | 0 | 11 | 14 | 70.0 |
| 0 | 0 | 1 | 2 | 0 | 3 | 15 | 75.0 |
| 4 | 1 | 1 | 1 | 0 | 7 | 16 | 80.0 |
| 1 | 1 | 1 | 7 | 0 | 10 | 17 | 85.0 |
| 1 | 0 | 1 | 2 | 0 | 4 | 18 | 90.0 |
| 4 | 1 | 0 | 1 | 0 | 6 | 19 | 95.0 |
| 15 | 11 | 3 | 11 | 0 | 40 | 20 | 100.0 |

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

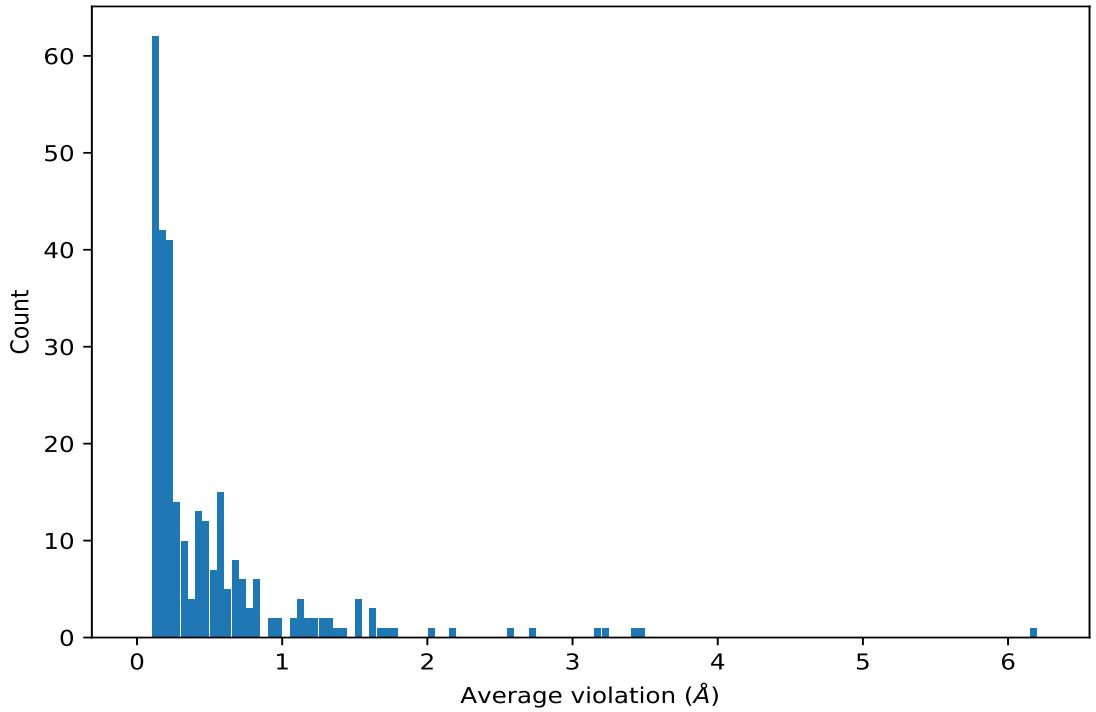
### 9.3.1 Bar graph : Distance violation statistics for the ensemble




## 9.4 Most violated distance restraints in the ensemble

### 9.4.1 Histogram : Distribution of mean distance violations

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




### 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[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 20 | 6.16 | 1.75 | 6.51 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 20 | 3.44 | 0.39 | 3.54 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 20 | 3.24 | 0.37 | 3.34 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 20 | 2.57 | 0.24 | 2.6 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 20 | 2.0 | 1.07 | 1.77 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 20 | 1.75 | 0.09 | 1.78 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 20 | 1.67 | 0.35 | 1.64 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 20 | 1.62 | 0.04 | 1.62 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 20 | 1.53 | 0.21 | 1.62 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 20 | 1.52 | 0.66 | 1.39 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 20 | 1.42 | 0.61 | 1.4 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 20 | 1.33 | 0.31 | 1.34 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 20 | 1.3 | 0.02 | 1.3 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 20 | 1.28 | 0.15 | 1.3 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 20 | 1.27 | 0.08 | 1.27 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 20 | 1.21 | 0.05 | 1.2 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 20 | 1.19 | 0.08 | 1.18 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 20 | 1.19 | 0.05 | 1.19 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 20 | 1.13 | 0.18 | 1.13 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 20 | 1.12 | 0.12 | 1.14 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 20 | 1.12 | 0.12 | 1.14 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 20 | 1.09 | 0.12 | 1.09 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 20 | 0.98 | 0.21 | 0.96 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 20 | 0.98 | 0.13 | 1.0 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 20 | 0.85 | 0.05 | 0.86 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 20 | 0.76 | 0.06 | 0.74 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 20 | 0.73 | 0.08 | 0.76 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 20 | 0.73 | 0.03 | 0.73 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 20 | 0.73 | 0.03 | 0.73 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 20 | 0.66 | 0.27 | 0.78 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 20 | 0.66 | 0.0 | 0.66 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 20 | 0.59 | 0.09 | 0.57 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 20 | 0.58 | 0.16 | 0.58 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 20 | 0.58 | 0.16 | 0.58 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 20 | 0.57 | 0.12 | 0.6 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 20 | 0.57 | 0.05 | 0.56 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 20 | 0.56 | 0.05 | 0.57 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 20 | 0.53 | 0.01 | 0.53 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 20 | 0.5 | 0.02 | 0.5 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 20 | 0.5 | 0.02 | 0.5 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 20 | 0.5 | 0.01 | 0.5 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 20 | 0.49 | 0.01 | 0.49 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 20 | 0.45 | 0.01 | 0.45 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 20 | 0.33 | 0.0 | 0.33 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 19 | 1.22 | 0.04 | 1.23 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 19 | 0.91 | 0.32 | 0.9 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 19 | 0.76 | 0.38 | 0.91 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 19 | 0.61 | 0.1 | 0.63 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 19 | 0.35 | 0.01 | 0.35 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 19 | 0.2 | 0.02 | 0.2 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 18 | 3.49 | 0.86 | 3.9 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 18 | 1.05 | 0.51 | 0.9 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 18 | 0.6 | 0.34 | 0.52 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 18 | 0.46 | 0.2 | 0.43 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 18 | 0.46 | 0.2 | 0.43 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 17 | 1.74 | 1.09 | 1.17 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 17 | 1.37 | 0.65 | 1.31 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 17 | 0.92 | 0.15 | 0.95 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 17 | 0.81 | 0.28 | 0.94 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 17 | 0.81 | 0.28 | 0.94 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 17 | 0.65 | 0.3 | 0.71 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 17 | 0.65 | 0.3 | 0.71 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 17 | 0.65 | 0.25 | 0.72 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 17 | 0.64 | 0.12 | 0.67 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 17 | 0.47 | 0.13 | 0.48 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 17 | 0.23 | 0.05 | 0.25 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 17 | 0.17 | 0.04 | 0.16 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 16 | 1.14 | 0.18 | 1.19 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 16 | 0.79 | 0.51 | 0.64 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 16 | 0.58 | 0.2 | 0.54 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 16 | 0.58 | 0.01 | 0.58 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 16 | 0.42 | 0.05 | 0.43 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 16 | 0.39 | 0.04 | 0.4 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 16 | 0.22 | 0.04 | 0.23 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 16 | 0.22 | 0.04 | 0.23 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 15 | 0.47 | 0.14 | 0.5 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 15 | 0.18 | 0.06 | 0.16 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 15 | 0.15 | 0.03 | 0.15 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 14 | 2.72 | 1.63 | 3.64 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 14 | 0.82 | 0.5 | 0.75 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 14 | 0.82 | 0.5 | 0.75 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 14 | 0.82 | 0.5 | 0.75 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 14 | 0.69 | 0.27 | 0.72 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 14 | 0.44 | 0.15 | 0.42 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 14 | 0.44 | 0.15 | 0.42 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 14 | 0.3 | 0.13 | 0.26 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 14 | 0.29 | 0.11 | 0.34 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 14 | 0.24 | 0.1 | 0.23 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 14 | 0.23 | 0.1 | 0.22 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 14 | 0.2 | 0.09 | 0.18 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 14 | 0.2 | 0.05 | 0.19 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 14 | 0.19 | 0.08 | 0.17 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 13 | 1.64 | 0.11 | 1.64 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 13 | 0.73 | 0.14 | 0.76 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 13 | 0.73 | 0.14 | 0.76 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 13 | 0.52 | 0.23 | 0.51 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 13 | 0.49 | 0.21 | 0.59 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 13 | 0.31 | 0.09 | 0.32 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 13 | 0.29 | 0.17 | 0.23 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 13 | 0.21 | 0.05 | 0.2 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 13 | 0.2 | 0.06 | 0.19 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 13 | 0.13 | 0.02 | 0.13 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 12 | 0.61 | 0.01 | 0.61 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 12 | 0.6 | 0.01 | 0.6 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 12 | 0.58 | 0.21 | 0.6 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 12 | 0.34 | 0.12 | 0.36 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 12 | 0.19 | 0.02 | 0.19 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 12 | 0.17 | 0.03 | 0.18 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 12 | 0.16 | 0.03 | 0.18 |
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 11 | 0.65 | 0.46 | 0.47 |
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 11 | 0.59 | 0.15 | 0.64 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 11 | 0.39 | 0.11 | 0.41 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 11 | 0.25 | 0.09 | 0.23 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 11 | 0.23 | 0.08 | 0.22 |
| (1,364) | 1:A:52:ARG:H | 1:A:75:PHE:HD2 | 10 | 3.16 | 0.15 | 3.16 |
| (1,443) | 1:A:60:ARG:HA | 1:A:67:THR:HG22 | 10 | 1.64 | 0.3 | 1.68 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG2 | 10 | 1.54 | 0.45 | 1.78 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG3 | 10 | 1.54 | 0.45 | 1.78 |
| (1,645) | 1:A:97:ALA:H | 1:A:97:ALA:HB3 | 10 | 0.67 | 0.3 | 0.72 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG13 | 10 | 0.6 | 0.47 | 0.44 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG12 | 10 | 0.6 | 0.47 | 0.44 |
| (1,388) | 1:A:53:TRP:H | 1:A:75:PHE:HD2 | 10 | 0.52 | 0.12 | 0.58 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD12 | 10 | 0.41 | 0.19 | 0.44 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD22 | 10 | 0.41 | 0.19 | 0.44 |
| (1,474) | 1:A:66:ARG:H | 1:A:67:THR:H | 10 | 0.25 | 0.08 | 0.25 |
| (1,626) | 1:A:92:GLN:HA | 1:A:93:ASP:H | 10 | 0.22 | 0.12 | 0.18 |
| (1,663) | 1:A:104:PHE:H | 1:A:105:GLY:H | 10 | 0.22 | 0.06 | 0.22 |
| (1,32) | 1:A:9:LYS:H | 1:A:10:GLN:HA | 10 | 0.16 | 0.04 | 0.16 |
| (1,521) | 1:A:73:THR:HG1 | 1:A:74:VAL:H | 10 | 0.14 | 0.02 | 0.14 |
| (1,147) | 1:A:25:GLN:H | 1:A:26:LEU:H | 10 | 0.14 | 0.03 | 0.13 |
| (1,681) | 1:A:109:ALA:H | 1:A:110:ARG:H | 9 | 0.32 | 0.16 | 0.32 |
| (1,696) | 1:A:112:LYS:H | 1:A:113:LYS:H | 9 | 0.25 | 0.09 | 0.27 |
| (1,705) | 1:A:115:GLN:HA | 1:A:116:ARG:H | 9 | 0.24 | 0.04 | 0.25 |
| (1,628) | 1:A:93:ASP:H | 1:A:94:GLU:H | 9 | 0.22 | 0.06 | 0.2 |
| (1,506) | 1:A:71:ASN:H | 1:A:72:PHE:H | 9 | 0.2 | 0.09 | 0.17 |
| (1,250) | 1:A:35:VAL:HG11 | 1:A:39:LEU:HD11 | 9 | 0.16 | 0.03 | 0.17 |
| (1,384) | 1:A:53:TRP:H | 1:A:73:THR:HA | 9 | 0.14 | 0.03 | 0.12 |
| (1,424) | 1:A:58:THR:H | 1:A:59:GLN:H | 9 | 0.13 | 0.02 | 0.12 |
| (1,423) | 1:A:58:THR:H | 1:A:58:THR:HG23 | 8 | 0.71 | 0.19 | 0.74 |
| (1,99) | 1:A:19:LYS:HA | 1:A:22:ALA:H | 8 | 0.42 | 0.28 | 0.3 |
| (1,68) | 1:A:15:GLY:H | 1:A:16:ASN:H | 8 | 0.38 | 0.14 | 0.39 |
| (1,335) | 1:A:46:ASP:HA | 1:A:48:PHE:H | 8 | 0.28 | 0.06 | 0.3 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,620) | 1:A:91:SER:H | 1:A:92:GLN:H | 8 | 0.22 | 0.13 | 0.18 |
| (1,345) | 1:A:49:HIS:HA | 1:A:49:HIS:HD2 | 8 | 0.22 | 0.09 | 0.2 |
| (1,111) | 1:A:21:ASN:HA | 1:A:24:GLU:H | 8 | 0.18 | 0.08 | 0.16 |
| (1,431) | 1:A:58:THR:HG1 | 1:A:59:GLN:H | 8 | 0.18 | 0.05 | 0.17 |
| (1,604) | 1:A:85:GLU:H | 1:A:86:GLY:H | 8 | 0.16 | 0.04 | 0.15 |
| (1,136) | 1:A:23:VAL:HG12 | 1:A:24:GLU:H | 8 | 0.16 | 0.02 | 0.16 |
| (1,137) | 1:A:23:VAL:HG12 | 1:A:24:GLU:HA | 8 | 0.16 | 0.04 | 0.15 |
| (1,597) | 1:A:83:ARG:HA | 1:A:84:TRP:H | 8 | 0.16 | 0.03 | 0.16 |
| (1,312) | 1:A:43:SER:H | 1:A:43:SER:HA | 8 | 0.13 | 0.01 | 0.13 |
| (1,228) | 1:A:34:GLN:H | 1:A:36:SER:H | 8 | 0.13 | 0.02 | 0.12 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB3 | 7 | 0.48 | 0.24 | 0.51 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB1 | 7 | 0.48 | 0.24 | 0.51 |
| (1,380) | 1:A:52:ARG:HG3 | 1:A:73:THR:HG22 | 7 | 0.33 | 0.11 | 0.34 |
| (1,665) | 1:A:104:PHE:HA | 1:A:105:GLY:H | 7 | 0.31 | 0.05 | 0.31 |
| (1,634) | 1:A:94:GLU:H | 1:A:95:GLN:H | 7 | 0.21 | 0.06 | 0.23 |
| (1,432) | 1:A:58:THR:HG22 | 1:A:59:GLN:H | 7 | 0.2 | 0.08 | 0.18 |
| (1,357) | 1:A:51:GLN:HA | 1:A:52:ARG:H | 7 | 0.2 | 0.1 | 0.15 |
| (1,273) | 1:A:37:ALA:HA | 1:A:41:THR:H | 7 | 0.17 | 0.05 | 0.16 |
| (1,193) | 1:A:30:GLN:H | 1:A:31:SER:H | 7 | 0.14 | 0.04 | 0.12 |
| (1,101) | 1:A:20:GLN:H | 1:A:20:GLN:HA | 7 | 0.14 | 0.03 | 0.12 |
| (1,28) | 1:A:8:TYR:H | 1:A:8:TYR:HA | 7 | 0.13 | 0.01 | 0.13 |
| (1,152) | 1:A:26:LEU:H | 1:A:26:LEU:HA | 7 | 0.13 | 0.02 | 0.13 |
| (1,573) | 1:A:79:GLU:H | 1:A:80:GLN:H | 7 | 0.12 | 0.01 | 0.11 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD12 | 6 | 0.45 | 0.19 | 0.38 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD22 | 6 | 0.45 | 0.19 | 0.38 |
| (1,635) | 1:A:94:GLU:HA | 1:A:95:GLN:H | 6 | 0.43 | 0.14 | 0.44 |
| (1,651) | 1:A:99:ALA:H | 1:A:99:ALA:HB2 | 6 | 0.31 | 0.18 | 0.26 |
| (1,477) | 1:A:67:THR:H | 1:A:67:THR:HB | 6 | 0.24 | 0.07 | 0.24 |
| (1,700) | 1:A:114:LYS:H | 1:A:115:GLN:H | 6 | 0.22 | 0.15 | 0.16 |
| (1,169) | 1:A:26:LEU:HD12 | 1:A:84:TRP:HE3 | 6 | 0.18 | 0.04 | 0.17 |
| (1,135) | 1:A:23:VAL:HG11 | 1:A:84:TRP:HD1 | 6 | 0.17 | 0.03 | 0.16 |
| (1,507) | 1:A:71:ASN:H | 1:A:88:TYR:HA | 6 | 0.17 | 0.04 | 0.16 |
| (1,42) | 1:A:11:PRO:HA | 1:A:12:ILE:H | 6 | 0.17 | 0.06 | 0.16 |
| (1,483) | 1:A:68:GLU:H | 1:A:69:ILE:H | 6 | 0.16 | 0.01 | 0.16 |
| (1,264) | 1:A:36:SER:HA | 1:A:53:TRP:HZ2 | 6 | 0.13 | 0.01 | 0.13 |
| (1,199) | 1:A:31:SER:H | 1:A:81:VAL:H | 6 | 0.12 | 0.01 | 0.12 |
| (1,413) | 1:A:56:THR:HG22 | 1:A:69:ILE:HG23 | 5 | 0.61 | 0.36 | 0.4 |
| (1,646) | 1:A:97:ALA:HA | 1:A:97:ALA:HB2 | 5 | 0.58 | 0.01 | 0.58 |
| (1,486) | 1:A:69:ILE:H | 1:A:69:ILE:HB | 5 | 0.48 | 0.27 | 0.34 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 5 | 0.42 | 0.15 | 0.48 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 5 | 0.42 | 0.15 | 0.48 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 5 | 0.42 | 0.15 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 5 | 0.42 | 0.15 | 0.48 |
| (1,323) | 1:A:44:ILE:HA | 1:A:44:ILE:HD12 | 5 | 0.36 | 0.28 | 0.15 |
| (1,630) | 1:A:93:ASP:HA | 1:A:94:GLU:H | 5 | 0.3 | 0.09 | 0.3 |
| (1,30) | 1:A:8:TYR:H | 1:A:9:LYS:H | 5 | 0.2 | 0.04 | 0.2 |
| (1,20) | 1:A:6:ILE:HA | 1:A:8:TYR:H | 5 | 0.17 | 0.06 | 0.13 |
| (1,403) | 1:A:55:TYR:H | 1:A:73:THR:HA | 5 | 0.15 | 0.03 | 0.15 |
| (1,644) | 1:A:97:ALA:H | 1:A:97:ALA:HA | 5 | 0.15 | 0.03 | 0.13 |
| (1,293) | 1:A:39:LEU:HD12 | 1:A:53:TRP:HH2 | 5 | 0.14 | 0.03 | 0.12 |
| (1,676) | 1:A:108:LEU:H | 1:A:108:LEU:HA | 5 | 0.14 | 0.01 | 0.13 |
| (1,52) | 1:A:12:ILE:HG23 | 1:A:13:TYR:H | 5 | 0.13 | 0.01 | 0.13 |
| (1,694) | 1:A:112:LYS:H | 1:A:112:LYS:HA | 5 | 0.13 | 0.01 | 0.13 |
| (1,43) | 1:A:12:ILE:H | 1:A:12:ILE:HA | 5 | 0.12 | 0.01 | 0.13 |
| (1,462) | 1:A:64:LEU:H | 1:A:64:LEU:HA | 5 | 0.12 | 0.01 | 0.11 |
| (1,448) | 1:A:61:VAL:H | 1:A:62:ASP:H | 4 | 0.43 | 0.09 | 0.42 |
| (1,661) | 1:A:103:GLN:H | 1:A:104:PHE:H | 4 | 0.34 | 0.14 | 0.38 |
| (1,427) | 1:A:58:THR:HA | 1:A:59:GLN:H | 4 | 0.27 | 0.04 | 0.26 |
| (1,349) | 1:A:50:ALA:H | 1:A:50:ALA:HB2 | 4 | 0.26 | 0.02 | 0.27 |
| (1,711) | 1:A:117:GLY:H | 1:A:118:ARG:H | 4 | 0.25 | 0.12 | 0.22 |
| (1,406) | 1:A:56:THR:H | 1:A:57:SER:H | 4 | 0.22 | 0.06 | 0.24 |
| (1,469) | 1:A:64:LEU:HD13 | 1:A:65:ALA:H | 4 | 0.19 | 0.07 | 0.18 |
| (1,704) | 1:A:115:GLN:H | 1:A:116:ARG:H | 4 | 0.18 | 0.06 | 0.18 |
| (1,16) | 1:A:6:ILE:H | 1:A:7:ILE:H | 4 | 0.18 | 0.08 | 0.16 |
| (1,336) | 1:A:47:PRO:HA | 1:A:50:ALA:H | 4 | 0.18 | 0.09 | 0.14 |
| (1,473) | 1:A:65:ALA:HB2 | 1:A:66:ARG:H | 4 | 0.18 | 0.04 | 0.16 |
| (1,58) | 1:A:14:GLN:H | 1:A:14:GLN:HA | 4 | 0.17 | 0.03 | 0.18 |
| (1,85) | 1:A:18:ILE:HA | 1:A:18:ILE:HG22 | 4 | 0.15 | 0.04 | 0.15 |
| (1,227) | 1:A:34:GLN:H | 1:A:35:VAL:H | 4 | 0.14 | 0.02 | 0.14 |
| (1,618) | 1:A:90:PRO:HA | 1:A:91:SER:H | 4 | 0.14 | 0.02 | 0.15 |
| (1,220) | 1:A:33:GLN:HA | 1:A:36:SER:H | 4 | 0.14 | 0.02 | 0.13 |
| (1,64) | 1:A:14:GLN:HA | 1:A:15:GLY:H | 4 | 0.13 | 0.01 | 0.13 |
| (1,554) | 1:A:76:PHE:HA | 1:A:81:VAL:HA | 4 | 0.13 | 0.02 | 0.12 |
| (1,53) | 1:A:13:TYR:H | 1:A:13:TYR:HA | 4 | 0.12 | 0.01 | 0.12 |
| (1,489) | 1:A:69:ILE:H | 1:A:69:ILE:HD12 | 3 | 2.18 | 0.03 | 2.19 |
| (1,194) | 1:A:30:GLN:H | 1:A:81:VAL:H | 3 | 0.53 | 0.45 | 0.29 |
| (1,407) | 1:A:56:THR:HA | 1:A:56:THR:HG1 | 3 | 0.31 | 0.11 | 0.34 |
| (1,456) | 1:A:62:ASP:HA | 1:A:63:ARG:H | 3 | 0.24 | 0.1 | 0.22 |
| (1,692) | 1:A:111:ASP:HA | 1:A:112:LYS:H | 3 | 0.22 | 0.07 | 0.21 |
| (1,678) | 1:A:108:LEU:H | 1:A:109:ALA:H | 3 | 0.22 | 0.09 | 0.17 |
| (1,490) | 1:A:69:ILE:HA | 1:A:69:ILE:HG13 | 3 | 0.22 | 0.04 | 0.21 |
| (1,490) | 1:A:69:ILE:HA | 1:A:69:ILE:HG12 | 3 | 0.22 | 0.04 | 0.21 |
| (1,652) | 1:A:99:ALA:H | 1:A:100:ALA:H | 3 | 0.22 | 0.05 | 0.2 |
| (1,66) | 1:A:14:GLN:HB2 | 1:A:15:GLY:H | 3 | 0.22 | 0.08 | 0.22 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,57) | 1:A:13:TYR:HA | 1:A:14:GLN:H | 3 | 0.21 | 0.07 | 0.25 |
| (1,512) | 1:A:72:PHE:HA | 1:A:87:ASP:H | 3 | 0.21 | 0.08 | 0.21 |
| (1,45) | 1:A:12:ILE:H | 1:A:13:TYR:H | 3 | 0.2 | 0.03 | 0.18 |
| (1,331) | 1:A:45:PRO:HA | 1:A:46:ASP:H | 3 | 0.18 | 0.05 | 0.21 |
| (1,594) | 1:A:83:ARG:H | 1:A:83:ARG:HE | 3 | 0.17 | 0.02 | 0.15 |
| (1,221) | 1:A:33:GLN:HA | 1:A:37:ALA:H | 3 | 0.16 | 0.03 | 0.15 |
| (1,65) | 1:A:14:GLN:HA | 1:A:16:ASN:H | 3 | 0.16 | 0.02 | 0.16 |
| (1,446) | 1:A:61:VAL:H | 1:A:61:VAL:HB | 3 | 0.16 | 0.05 | 0.14 |
| (1,640) | 1:A:96:LEU:H | 1:A:96:LEU:HA | 3 | 0.16 | 0.0 | 0.16 |
| (1,2) | 1:A:2:ALA:H | 1:A:3:GLY:H | 3 | 0.16 | 0.03 | 0.16 |
| (1,552) | 1:A:76:PHE:HA | 1:A:78:ASN:H | 3 | 0.15 | 0.02 | 0.16 |
| (1,622) | 1:A:91:SER:HA | 1:A:92:GLN:H | 3 | 0.15 | 0.03 | 0.17 |
| (1,648) | 1:A:98:LYS:HA | 1:A:99:ALA:H | 3 | 0.15 | 0.01 | 0.14 |
| (1,439) | 1:A:60:ARG:H | 1:A:61:VAL:H | 3 | 0.15 | 0.01 | 0.15 |
| (1,208) | 1:A:32:LYS:H | 1:A:33:GLN:H | 3 | 0.14 | 0.01 | 0.14 |
| (1,632) | 1:A:94:GLU:H | 1:A:94:GLU:HA | 3 | 0.14 | 0.01 | 0.15 |
| (1,120) | 1:A:22:ALA:HA | 1:A:26:LEU:H | 3 | 0.14 | 0.02 | 0.13 |
| (1,699) | 1:A:113:LYS:HA | 1:A:114:LYS:H | 3 | 0.14 | 0.01 | 0.14 |
| (1,536) | 1:A:74:VAL:HG21 | 1:A:84:TRP:HZ3 | 3 | 0.14 | 0.01 | 0.14 |
| (1,566) | 1:A:77:GLU:H | 1:A:81:VAL:HA | 3 | 0.14 | 0.02 | 0.12 |
| (1,211) | 1:A:32:LYS:HA | 1:A:35:VAL:H | 3 | 0.13 | 0.02 | 0.12 |
| (1,588) | 1:A:82:VAL:H | 1:A:83:ARG:H | 3 | 0.12 | 0.02 | 0.11 |
| (1,587) | 1:A:81:VAL:HG11 | 1:A:82:VAL:HA | 3 | 0.12 | 0.01 | 0.11 |
| (1,243) | 1:A:35:VAL:HA | 1:A:37:ALA:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,650) | 1:A:99:ALA:H | 1:A:99:ALA:HA | 3 | 0.11 | 0.0 | 0.11 |
| (1,309) | 1:A:41:THR:HG23 | 1:A:53:TRP:HD1 | 2 | 0.62 | 0.31 | 0.62 |
| (1,524) | 1:A:73:THR:HG22 | 1:A:75:PHE:HE1 | 2 | 0.42 | 0.2 | 0.42 |
| (1,420) | 1:A:57:SER:HA | 1:A:58:THR:H | 2 | 0.29 | 0.18 | 0.29 |
| (1,395) | 1:A:54:ASP:HA | 1:A:55:TYR:H | 2 | 0.26 | 0.09 | 0.26 |
| (1,497) | 1:A:69:ILE:HG22 | 1:A:70:LYS:H | 2 | 0.25 | 0.09 | 0.25 |
| (1,61) | 1:A:14:GLN:H | 1:A:15:GLY:H | 2 | 0.24 | 0.12 | 0.24 |
| (1,12) | 1:A:5:GLY:H | 1:A:6:ILE:H | 2 | 0.23 | 0.05 | 0.23 |
| (1,463) | 1:A:64:LEU:H | 1:A:64:LEU:HG | 2 | 0.22 | 0.02 | 0.22 |
| (1,504) | 1:A:70:LYS:HA | 1:A:89:PHE:H | 2 | 0.22 | 0.1 | 0.22 |
| (1,114) | 1:A:22:ALA:H | 1:A:23:VAL:H | 2 | 0.21 | 0.03 | 0.21 |
| (1,322) | 1:A:44:ILE:HA | 1:A:44:ILE:HG22 | 2 | 0.21 | 0.1 | 0.21 |
| (1,303) | 1:A:41:THR:HA | 1:A:41:THR:HG1 | 2 | 0.18 | 0.06 | 0.18 |
| (1,441) | 1:A:60:ARG:HA | 1:A:61:VAL:H | 2 | 0.17 | 0.0 | 0.17 |
| (1,175) | 1:A:27:GLN:H | 1:A:28:VAL:H | 2 | 0.17 | 0.01 | 0.17 |
| (1,109) | 1:A:21:ASN:H | 1:A:23:VAL:H | 2 | 0.16 | 0.04 | 0.16 |
| (1,470) | 1:A:65:ALA:H | 1:A:65:ALA:HB2 | 2 | 0.16 | 0.04 | 0.16 |
| (1,470) | 1:A:65:ALA:H | 1:A:65:ALA:HB3 | 2 | 0.16 | 0.04 | 0.16 |

*Continued on next page...*

*Continued from previous page...*

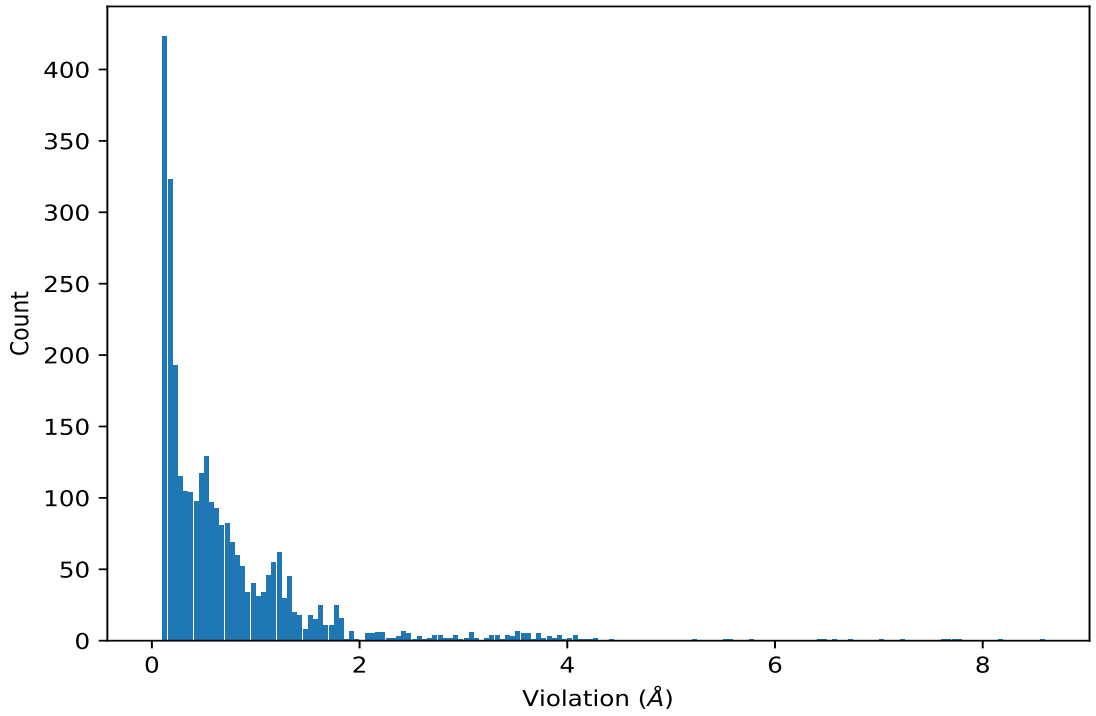
| Key | Atom-1 | Atom-2 | Models[1] | Mean (Å) | SD[1] (Å) | Median (Å) |
|---|---|---|---|---|---|---|
| (1,623) | 1:A:92:GLN:H | 1:A:93:ASP:H | 2 | 0.16 | 0.01 | 0.16 |
| (1,62) | 1:A:14:GLN:HA | 1:A:14:GLN:HB2 | 2 | 0.16 | 0.02 | 0.16 |
| (1,421) | 1:A:57:SER:HA | 1:A:58:THR:HB | 2 | 0.15 | 0.03 | 0.15 |
| (1,555) | 1:A:76:PHE:HA | 1:A:82:VAL:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,685) | 1:A:110:ARG:H | 1:A:111:ASP:H | 2 | 0.14 | 0.0 | 0.14 |
| (1,110) | 1:A:21:ASN:H | 1:A:24:GLU:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,161) | 1:A:26:LEU:HA | 1:A:28:VAL:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,360) | 1:A:52:ARG:H | 1:A:52:ARG:HA | 2 | 0.14 | 0.01 | 0.14 |
| (1,697) | 1:A:112:LYS:HA | 1:A:113:LYS:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,298) | 1:A:40:GLY:H | 1:A:41:THR:H | 2 | 0.13 | 0.01 | 0.13 |
| (1,286) | 1:A:39:LEU:H | 1:A:39:LEU:HG | 2 | 0.12 | 0.02 | 0.12 |
| (1,670) | 1:A:106:ARG:H | 1:A:107:ASN:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,91) | 1:A:18:ILE:HD12 | 1:A:23:VAL:HG11 | 2 | 0.12 | 0.0 | 0.12 |
| (1,91) | 1:A:18:ILE:HD12 | 1:A:23:VAL:HG22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,209) | 1:A:32:LYS:H | 1:A:34:GLN:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,494) | 1:A:69:ILE:HB | 1:A:69:ILE:HD12 | 2 | 0.12 | 0.0 | 0.12 |
| (1,122) | 1:A:23:VAL:H | 1:A:23:VAL:HB | 2 | 0.11 | 0.0 | 0.11 |
| (1,310) | 1:A:42:PRO:HA | 1:A:43:SER:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,405) | 1:A:56:THR:H | 1:A:56:THR:HB | 2 | 0.11 | 0.0 | 0.11 |

[1]Number of violated models, [2]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) |
|---|---|---|---|---|
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 16 | 8.6 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 4 | 8.16 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 7 | 7.79 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 9 | 7.7 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 13 | 7.67 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 2 | 7.61 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 10 | 7.24 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 8 | 7.03 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 18 | 6.74 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 11 | 6.57 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 6 | 6.45 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 3 | 6.41 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 15 | 5.75 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 14 | 5.57 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 12 | 5.54 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 19 | 5.2 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 3 | 4.4 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 7 | 4.28 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 4 | 4.27 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 17 | 4.2 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 3 | 4.17 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 5 | 4.11 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 18 | 4.07 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 5 | 4.05 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 20 | 4.05 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 19 | 4.05 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 8 | 4.04 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 16 | 4.02 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 10 | 3.97 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 19 | 3.93 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 10 | 3.92 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 16 | 3.9 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 11 | 3.9 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 2 | 3.89 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 4 | 3.86 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 3 | 3.82 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 6 | 3.82 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 14 | 3.82 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 17 | 3.78 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 11 | 3.76 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 15 | 3.74 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 5 | 3.72 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 13 | 3.71 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 20 | 3.7 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 10 | 3.7 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 15 | 3.67 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 6 | 3.64 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 7 | 3.64 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 2 | 3.6 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 3 | 3.6 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 11 | 3.6 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 20 | 3.59 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 17 | 3.59 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 6 | 3.58 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 12 | 3.58 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 11 | 3.56 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 14 | 3.54 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 13 | 3.54 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 10 | 3.53 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 15 | 3.53 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 1 | 3.51 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 4 | 3.51 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 19 | 3.5 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 20 | 3.48 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 18 | 3.47 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 17 | 3.46 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 5 | 3.44 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 2 | 3.43 |
| (1,364) | 1:A:52:ARG:H | 1:A:75:PHE:HD2 | 11 | 3.4 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 15 | 3.4 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 10 | 3.38 |
| (1,364) | 1:A:52:ARG:H | 1:A:75:PHE:HD2 | 3 | 3.31 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 8 | 3.31 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 17 | 3.3 |
| (1,364) | 1:A:52:ARG:H | 1:A:75:PHE:HD2 | 17 | 3.3 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 4 | 3.29 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 12 | 3.29 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 9 | 3.26 |
| (1,364) | 1:A:52:ARG:H | 1:A:75:PHE:HD2 | 12 | 3.26 |
| (1,364) | 1:A:52:ARG:H | 1:A:75:PHE:HD2 | 20 | 3.24 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 1 | 3.22 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 7 | 3.11 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 7 | 3.1 |
| (1,364) | 1:A:52:ARG:H | 1:A:75:PHE:HD2 | 10 | 3.09 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 19 | 3.08 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 7 | 3.07 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 16 | 3.07 |
| (1,364) | 1:A:52:ARG:H | 1:A:75:PHE:HD2 | 4 | 3.05 |
| (1,364) | 1:A:52:ARG:H | 1:A:75:PHE:HD2 | 19 | 3.05 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 9 | 3.04 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 19 | 3.04 |
| (1,364) | 1:A:52:ARG:H | 1:A:75:PHE:HD2 | 18 | 2.97 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 12 | 2.94 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 12 | 2.93 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 6 | 2.93 |
| (1,364) | 1:A:52:ARG:H | 1:A:75:PHE:HD2 | 6 | 2.92 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 8 | 2.89 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 3 | 2.88 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 12 | 2.84 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 8 | 2.82 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 11 | 2.78 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 6 | 2.78 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 9 | 2.76 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 2 | 2.76 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 15 | 2.73 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 1 | 2.72 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 10 | 2.72 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 7 | 2.7 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 18 | 2.68 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 16 | 2.67 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 19 | 2.64 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 4 | 2.59 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 14 | 2.56 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 11 | 2.55 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 9 | 2.54 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 19 | 2.49 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 14 | 2.48 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 17 | 2.47 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 13 | 2.47 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 17 | 2.45 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 13 | 2.43 |
| (1,513) | 1:A:72:PHE:HE1 | 1:A:74:VAL:HG21 | 18 | 2.43 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 3 | 2.42 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 1 | 2.42 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 20 | 2.42 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 20 | 2.41 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 20 | 2.4 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 8 | 2.37 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 7 | 2.36 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 17 | 2.35 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 5 | 2.33 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 4 | 2.32 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 10 | 2.25 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 4 | 2.25 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 13 | 2.24 |
| (1,392) | 1:A:53:TRP:HH2 | 1:A:72:PHE:HE1 | 12 | 2.23 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 11 | 2.23 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 20 | 2.22 |
| (1,489) | 1:A:69:ILE:H | 1:A:69:ILE:HD12 | 12 | 2.21 |
| (1,139) | 1:A:23:VAL:HG23 | 1:A:72:PHE:HE2 | 18 | 2.21 |
| (1,489) | 1:A:69:ILE:H | 1:A:69:ILE:HD12 | 19 | 2.19 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 10 | 2.19 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 12 | 2.19 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 12 | 2.18 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 3 | 2.18 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 11 | 2.16 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 17 | 2.14 |
| (1,489) | 1:A:69:ILE:H | 1:A:69:ILE:HD12 | 5 | 2.13 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 18 | 2.13 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 6 | 2.1 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 3 | 2.1 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 4 | 2.09 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG2 | 4 | 2.08 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG3 | 4 | 2.08 |
| (1,443) | 1:A:60:ARG:HA | 1:A:67:THR:HG22 | 7 | 2.07 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 17 | 2.05 |
| (1,443) | 1:A:60:ARG:HA | 1:A:67:THR:HG22 | 8 | 1.96 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 5 | 1.92 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG2 | 12 | 1.92 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG3 | 12 | 1.92 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG2 | 3 | 1.91 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG3 | 3 | 1.91 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 18 | 1.91 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 5 | 1.9 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 12 | 1.86 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG2 | 17 | 1.84 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG3 | 17 | 1.84 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 6 | 1.84 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 19 | 1.84 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 14 | 1.83 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 2 | 1.83 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 20 | 1.83 |
| (1,443) | 1:A:60:ARG:HA | 1:A:67:THR:HG22 | 18 | 1.82 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 19 | 1.82 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 17 | 1.82 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 14 | 1.81 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 11 | 1.81 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG2 | 6 | 1.8 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG3 | 6 | 1.8 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 7 | 1.8 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 18 | 1.8 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 9 | 1.79 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 9 | 1.79 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 12 | 1.79 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 19 | 1.79 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 20 | 1.79 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 4 | 1.78 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 6 | 1.78 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 13 | 1.78 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 15 | 1.78 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 15 | 1.77 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 10 | 1.77 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 17 | 1.77 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 19 | 1.76 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG2 | 10 | 1.76 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG3 | 10 | 1.76 |
| (1,443) | 1:A:60:ARG:HA | 1:A:67:THR:HG22 | 11 | 1.76 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 4 | 1.76 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 14 | 1.76 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 13 | 1.76 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 17 | 1.75 |
| (1,443) | 1:A:60:ARG:HA | 1:A:67:THR:HG22 | 6 | 1.75 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 5 | 1.75 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 1 | 1.75 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 3 | 1.75 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 15 | 1.75 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 18 | 1.73 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 13 | 1.72 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 5 | 1.72 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 1 | 1.72 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 14 | 1.71 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 16 | 1.71 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 13 | 1.71 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 6 | 1.7 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 6 | 1.7 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 11 | 1.7 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 12 | 1.7 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 3 | 1.69 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 6 | 1.69 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 6 | 1.69 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 8 | 1.69 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 15 | 1.68 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 4 | 1.67 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 3 | 1.66 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 2 | 1.66 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 3 | 1.66 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 2 | 1.66 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 14 | 1.65 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 18 | 1.64 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 20 | 1.64 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 10 | 1.64 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 9 | 1.64 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 11 | 1.63 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 1 | 1.63 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 16 | 1.63 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 7 | 1.63 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 10 | 1.63 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 13 | 1.63 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 12 | 1.63 |
| (1,443) | 1:A:60:ARG:HA | 1:A:67:THR:HG22 | 19 | 1.62 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 20 | 1.62 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 1 | 1.62 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 8 | 1.62 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 11 | 1.62 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 15 | 1.62 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 4 | 1.62 |
| (1,443) | 1:A:60:ARG:HA | 1:A:67:THR:HG22 | 14 | 1.61 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 20 | 1.61 |
| (1,294) | 1:A:39:LEU:HD12 | 1:A:88:TYR:HE1 | 8 | 1.6 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 2 | 1.6 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 5 | 1.6 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 12 | 1.6 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 18 | 1.6 |
| (1,443) | 1:A:60:ARG:HA | 1:A:67:THR:HG22 | 13 | 1.59 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 10 | 1.59 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 1 | 1.58 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 10 | 1.58 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 10 | 1.58 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 10 | 1.58 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 1 | 1.58 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 3 | 1.58 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 9 | 1.57 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 4 | 1.57 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 17 | 1.56 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 19 | 1.56 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 17 | 1.55 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 2 | 1.55 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 12 | 1.55 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 19 | 1.54 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 11 | 1.54 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 11 | 1.54 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 11 | 1.54 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 10 | 1.54 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 15 | 1.54 |
| (1,253) | 1:A:35:VAL:HG22 | 1:A:36:SER:HA | 4 | 1.54 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 5 | 1.53 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 19 | 1.53 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 20 | 1.53 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 12 | 1.53 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 2 | 1.53 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 5 | 1.53 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 16 | 1.52 |
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 12 | 1.51 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 5 | 1.51 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG13 | 5 | 1.5 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG12 | 5 | 1.5 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 6 | 1.47 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 3 | 1.47 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 9 | 1.46 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 17 | 1.46 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 1 | 1.46 |
| (1,296) | 1:A:39:LEU:HD23 | 1:A:89:PHE:HD1 | 1 | 1.45 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 11 | 1.45 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 6 | 1.45 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 2 | 1.44 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 17 | 1.44 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 17 | 1.44 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 17 | 1.44 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 1 | 1.44 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 15 | 1.44 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 2 | 1.44 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 5 | 1.43 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 2 | 1.42 |
| (1,556) | 1:A:76:PHE:HA | 1:A:82:VAL:HG23 | 16 | 1.41 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 18 | 1.41 |
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 19 | 1.41 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 5 | 1.41 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 19 | 1.41 |
| (1,237) | 1:A:34:GLN:HB2 | 1:A:37:ALA:HB2 | 16 | 1.41 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 8 | 1.4 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 17 | 1.4 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 13 | 1.4 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 7 | 1.39 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 7 | 1.39 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 7 | 1.39 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 4 | 1.39 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 13 | 1.39 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 20 | 1.38 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 7 | 1.37 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 2 | 1.37 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 5 | 1.37 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 11 | 1.37 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 4 | 1.37 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 15 | 1.36 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 18 | 1.36 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 12 | 1.36 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 5 | 1.36 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 7 | 1.36 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 1 | 1.35 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 20 | 1.35 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 9 | 1.35 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 5 | 1.35 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG13 | 12 | 1.34 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG12 | 12 | 1.34 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 3 | 1.34 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 6 | 1.34 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 18 | 1.34 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 1 | 1.33 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 16 | 1.33 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 12 | 1.33 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 4 | 1.33 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 17 | 1.33 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 15 | 1.33 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 10 | 1.33 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 6 | 1.33 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 15 | 1.33 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 16 | 1.33 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 3 | 1.32 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 19 | 1.32 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 11 | 1.32 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 9 | 1.32 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 19 | 1.32 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 6 | 1.32 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 17 | 1.32 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 19 | 1.32 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 7 | 1.32 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 15 | 1.32 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 3 | 1.32 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 3 | 1.32 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 18 | 1.31 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 1 | 1.31 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 5 | 1.31 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 12 | 1.31 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 13 | 1.31 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 13 | 1.31 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 12 | 1.3 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 4 | 1.3 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 8 | 1.3 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 10 | 1.3 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 14 | 1.3 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 18 | 1.3 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 19 | 1.3 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 4 | 1.3 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 7 | 1.3 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 7 | 1.3 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 18 | 1.3 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 8 | 1.3 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 10 | 1.29 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 7 | 1.29 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 9 | 1.29 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 18 | 1.29 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 2 | 1.29 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 7 | 1.28 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 1 | 1.28 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 12 | 1.28 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 17 | 1.28 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 19 | 1.28 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 16 | 1.28 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 8 | 1.27 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 12 | 1.27 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 9 | 1.27 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 4 | 1.27 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 6 | 1.27 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 11 | 1.27 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 14 | 1.27 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 2 | 1.27 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 11 | 1.27 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 12 | 1.27 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 8 | 1.27 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 15 | 1.26 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 20 | 1.26 |
| (1,274) | 1:A:37:ALA:HB2 | 1:A:38:LEU:H | 20 | 1.26 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 2 | 1.25 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 3 | 1.25 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 20 | 1.25 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 8 | 1.25 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 12 | 1.25 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 4 | 1.24 |
| (1,645) | 1:A:97:ALA:H | 1:A:97:ALA:HB3 | 9 | 1.24 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 13 | 1.24 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 8 | 1.24 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 6 | 1.24 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 1 | 1.24 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 3 | 1.24 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 5 | 1.24 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 6 | 1.24 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 18 | 1.24 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 2 | 1.24 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 17 | 1.24 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 18 | 1.24 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 18 | 1.24 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 4 | 1.23 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 5 | 1.23 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 13 | 1.23 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG2 | 20 | 1.23 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG3 | 20 | 1.23 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 5 | 1.23 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 2 | 1.23 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 4 | 1.23 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 19 | 1.23 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 3 | 1.23 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 9 | 1.23 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 13 | 1.23 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 15 | 1.22 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 8 | 1.22 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 16 | 1.22 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 8 | 1.22 |
| (1,443) | 1:A:60:ARG:HA | 1:A:67:THR:HG22 | 3 | 1.22 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 10 | 1.22 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 13 | 1.22 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 19 | 1.22 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 1 | 1.22 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 1 | 1.22 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 5 | 1.21 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 2 | 1.21 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 17 | 1.21 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 5 | 1.21 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 18 | 1.21 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 8 | 1.21 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 7 | 1.21 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 17 | 1.21 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 15 | 1.21 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 11 | 1.21 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 11 | 1.21 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 3 | 1.2 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 3 | 1.2 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 13 | 1.2 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 6 | 1.2 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 15 | 1.2 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 18 | 1.2 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 20 | 1.2 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG2 | 11 | 1.2 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG3 | 11 | 1.2 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 3 | 1.2 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 19 | 1.2 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 9 | 1.2 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 11 | 1.2 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 5 | 1.2 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 5 | 1.2 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 9 | 1.19 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 10 | 1.19 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 10 | 1.19 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 11 | 1.19 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 15 | 1.19 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 16 | 1.19 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 20 | 1.19 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 7 | 1.19 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 9 | 1.19 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 20 | 1.19 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 10 | 1.19 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 8 | 1.18 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 14 | 1.18 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 1 | 1.18 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 2 | 1.18 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 3 | 1.18 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 3 | 1.18 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 11 | 1.18 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 7 | 1.18 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 9 | 1.18 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 10 | 1.18 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 12 | 1.18 |
| (1,342) | 1:A:48:PHE:HB2 | 1:A:49:HIS:H | 16 | 1.18 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 16 | 1.18 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 8 | 1.18 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 19 | 1.18 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 6 | 1.17 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 14 | 1.17 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 19 | 1.17 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 20 | 1.17 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 7 | 1.17 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 6 | 1.17 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 1 | 1.17 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 14 | 1.17 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 18 | 1.17 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 2 | 1.17 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 9 | 1.17 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 9 | 1.17 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 11 | 1.16 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 3 | 1.16 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 7 | 1.16 |
| (1,194) | 1:A:30:GLN:H | 1:A:81:VAL:H | 17 | 1.16 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 16 | 1.16 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 16 | 1.16 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 17 | 1.16 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 17 | 1.16 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 15 | 1.15 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 16 | 1.15 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 1 | 1.15 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 17 | 1.15 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 20 | 1.15 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 14 | 1.15 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 10 | 1.15 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 10 | 1.15 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 10 | 1.15 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 5 | 1.14 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 11 | 1.14 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 13 | 1.14 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 14 | 1.14 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 7 | 1.14 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 14 | 1.14 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 1 | 1.14 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 4 | 1.14 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 17 | 1.14 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 2 | 1.14 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 2 | 1.14 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 4 | 1.14 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 4 | 1.14 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 2 | 1.13 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 10 | 1.13 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 4 | 1.13 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 6 | 1.13 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 9 | 1.13 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 16 | 1.13 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 16 | 1.12 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 19 | 1.12 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 2 | 1.12 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 8 | 1.12 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 1 | 1.12 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 12 | 1.12 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 12 | 1.12 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 15 | 1.12 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 15 | 1.12 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 10 | 1.11 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 11 | 1.11 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 11 | 1.11 |
| (1,59) | 1:A:14:GLN:H | 1:A:14:GLN:HB2 | 11 | 1.11 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 12 | 1.11 |
| (1,580) | 1:A:80:GLN:HB3 | 1:A:81:VAL:H | 14 | 1.11 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 16 | 1.11 |
| (1,413) | 1:A:56:THR:HG22 | 1:A:69:ILE:HG23 | 20 | 1.11 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 7 | 1.11 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 7 | 1.11 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 20 | 1.1 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 20 | 1.1 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 8 | 1.1 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 12 | 1.1 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 19 | 1.1 |
| (1,327) | 1:A:44:ILE:HB | 1:A:44:ILE:HD12 | 11 | 1.1 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 13 | 1.1 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 13 | 1.1 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 6 | 1.09 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 6 | 1.09 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 14 | 1.09 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 1 | 1.09 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 3 | 1.09 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 2 | 1.09 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 19 | 1.09 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 17 | 1.09 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 10 | 1.09 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 19 | 1.09 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 19 | 1.09 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 1 | 1.08 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 4 | 1.08 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 1 | 1.08 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 16 | 1.08 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 2 | 1.08 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 17 | 1.08 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 7 | 1.08 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 16 | 1.08 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 9 | 1.08 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 20 | 1.08 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 20 | 1.08 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 5 | 1.07 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 1 | 1.07 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 16 | 1.07 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 15 | 1.06 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 15 | 1.06 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 15 | 1.06 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 6 | 1.06 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 18 | 1.05 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 2 | 1.05 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 14 | 1.05 |
| (1,443) | 1:A:60:ARG:HA | 1:A:67:THR:HG22 | 17 | 1.05 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 17 | 1.05 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 11 | 1.04 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 16 | 1.04 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 5 | 1.04 |
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 5 | 1.04 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 15 | 1.04 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 12 | 1.03 |
| (1,543) | 1:A:75:PHE:HB3 | 1:A:83:ARG:H | 18 | 1.03 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 12 | 1.03 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 1 | 1.03 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 14 | 1.03 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 14 | 1.03 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 11 | 1.02 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 6 | 1.02 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 9 | 1.02 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 13 | 1.02 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 20 | 1.02 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 12 | 1.02 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 9 | 1.02 |
| (1,27) | 1:A:7:ILE:HD11 | 1:A:8:TYR:H | 8 | 1.02 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 17 | 1.01 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 19 | 1.01 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 17 | 1.01 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 5 | 1.01 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 10 | 1.01 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 8 | 1.01 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 8 | 1.01 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 8 | 1.0 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 8 | 1.0 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 19 | 1.0 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 7 | 1.0 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 15 | 1.0 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 13 | 0.99 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 12 | 0.99 |
| (1,423) | 1:A:58:THR:H | 1:A:58:THR:HG23 | 14 | 0.99 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 13 | 0.99 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 9 | 0.98 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 2 | 0.98 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 2 | 0.98 |
| (1,257) | 1:A:35:VAL:HG21 | 1:A:76:PHE:HE1 | 11 | 0.98 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 4 | 0.98 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 20 | 0.98 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 6 | 0.97 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 10 | 0.97 |
| (1,413) | 1:A:56:THR:HG22 | 1:A:69:ILE:HG23 | 12 | 0.97 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 9 | 0.97 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 18 | 0.96 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 9 | 0.96 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 9 | 0.96 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 9 | 0.96 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 13 | 0.96 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 1 | 0.96 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 5 | 0.96 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 5 | 0.96 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 16 | 0.96 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 19 | 0.96 |
| (1,99) | 1:A:19:LYS:HA | 1:A:22:ALA:H | 3 | 0.95 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 14 | 0.95 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 14 | 0.95 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 15 | 0.95 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 15 | 0.95 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 3 | 0.95 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 18 | 0.95 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 4 | 0.95 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 6 | 0.95 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 18 | 0.95 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 13 | 0.95 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 8 | 0.95 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 8 | 0.95 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 16 | 0.95 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 16 | 0.95 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 11 | 0.95 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 10 | 0.94 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 10 | 0.94 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 16 | 0.94 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 16 | 0.94 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 12 | 0.94 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 14 | 0.94 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 3 | 0.94 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 7 | 0.94 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 16 | 0.94 |
| (1,309) | 1:A:41:THR:HG23 | 1:A:53:TRP:HD1 | 20 | 0.94 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 13 | 0.93 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 7 | 0.93 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 17 | 0.93 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 17 | 0.93 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 18 | 0.93 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 7 | 0.92 |
| (1,486) | 1:A:69:ILE:H | 1:A:69:ILE:HB | 12 | 0.92 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 19 | 0.92 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 15 | 0.92 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 5 | 0.92 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 8 | 0.92 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 11 | 0.92 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 3 | 0.91 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 4 | 0.91 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 4 | 0.91 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 16 | 0.91 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 19 | 0.9 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 1 | 0.9 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 6 | 0.9 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 2 | 0.9 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 6 | 0.9 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 15 | 0.9 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 12 | 0.9 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 14 | 0.9 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 6 | 0.89 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 2 | 0.89 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 2 | 0.89 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 4 | 0.89 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 8 | 0.89 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 10 | 0.89 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 10 | 0.89 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 3 | 0.89 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 12 | 0.89 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 17 | 0.88 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 17 | 0.88 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 2 | 0.88 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 6 | 0.88 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 9 | 0.88 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 14 | 0.88 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 15 | 0.88 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 19 | 0.88 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 4 | 0.88 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 13 | 0.88 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 9 | 0.88 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD12 | 9 | 0.87 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD22 | 9 | 0.87 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 2 | 0.87 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 4 | 0.87 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 17 | 0.87 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 4 | 0.87 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 4 | 0.87 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 17 | 0.87 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 12 | 0.86 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 15 | 0.86 |
| (1,645) | 1:A:97:ALA:H | 1:A:97:ALA:HB3 | 12 | 0.86 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 7 | 0.86 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 10 | 0.86 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 20 | 0.86 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 8 | 0.86 |
| (1,423) | 1:A:58:THR:H | 1:A:58:THR:HG23 | 13 | 0.86 |
| (1,423) | 1:A:58:THR:H | 1:A:58:THR:HG23 | 17 | 0.86 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 20 | 0.86 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 7 | 0.86 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 8 | 0.86 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 2 | 0.86 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 2 | 0.86 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 4 | 0.86 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 1 | 0.86 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 10 | 0.86 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 14 | 0.85 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 8 | 0.85 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 11 | 0.85 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG2 | 19 | 0.85 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG3 | 19 | 0.85 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 15 | 0.85 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 10 | 0.85 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 17 | 0.84 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 18 | 0.84 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 18 | 0.84 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 1 | 0.84 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 20 | 0.84 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 20 | 0.84 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 15 | 0.84 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 13 | 0.84 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 3 | 0.84 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 9 | 0.84 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 17 | 0.84 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 17 | 0.84 |
| (1,134) | 1:A:23:VAL:HG11 | 1:A:72:PHE:HD2 | 9 | 0.84 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 19 | 0.83 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 16 | 0.83 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 4 | 0.83 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 19 | 0.83 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 19 | 0.83 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 11 | 0.83 |
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 3 | 0.83 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 4 | 0.83 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 3 | 0.83 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 8 | 0.83 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 3 | 0.83 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 14 | 0.83 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 14 | 0.83 |
| (1,99) | 1:A:19:LYS:HA | 1:A:22:ALA:H | 12 | 0.82 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 13 | 0.82 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 13 | 0.82 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 9 | 0.82 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 4 | 0.82 |
| (1,645) | 1:A:97:ALA:H | 1:A:97:ALA:HB3 | 1 | 0.82 |
| (1,645) | 1:A:97:ALA:H | 1:A:97:ALA:HB3 | 8 | 0.82 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 16 | 0.82 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 19 | 0.82 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 20 | 0.82 |
| (1,254) | 1:A:35:VAL:HG22 | 1:A:53:TRP:HZ3 | 18 | 0.82 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB3 | 20 | 0.82 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB1 | 20 | 0.82 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 7 | 0.81 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 17 | 0.81 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 17 | 0.81 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 1 | 0.81 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 18 | 0.81 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 14 | 0.81 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 9 | 0.81 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 6 | 0.81 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 9 | 0.8 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 15 | 0.8 |
| (1,598) | 1:A:83:ARG:HB3 | 1:A:84:TRP:H | 10 | 0.8 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 2 | 0.8 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 6 | 0.8 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 19 | 0.8 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 16 | 0.8 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 2 | 0.8 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 14 | 0.8 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 1 | 0.8 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 16 | 0.8 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 5 | 0.8 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 5 | 0.8 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 2 | 0.79 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 13 | 0.79 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 14 | 0.79 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 15 | 0.79 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 10 | 0.79 |
| (1,645) | 1:A:97:ALA:H | 1:A:97:ALA:HB3 | 16 | 0.79 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 15 | 0.79 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 15 | 0.79 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 18 | 0.79 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG2 | 18 | 0.79 |
| (1,546) | 1:A:75:PHE:HD1 | 1:A:83:ARG:HG3 | 18 | 0.79 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 6 | 0.79 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 17 | 0.79 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 16 | 0.79 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 16 | 0.79 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 16 | 0.79 |
| (1,256) | 1:A:35:VAL:HG23 | 1:A:81:VAL:HG23 | 8 | 0.79 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG13 | 6 | 0.79 |
| (1,123) | 1:A:23:VAL:H | 1:A:23:VAL:HG22 | 6 | 0.79 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 10 | 0.78 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 20 | 0.78 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 1 | 0.78 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 1 | 0.78 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 9 | 0.78 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 17 | 0.78 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 18 | 0.78 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 14 | 0.78 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 3 | 0.78 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 18 | 0.77 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 18 | 0.77 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 16 | 0.77 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 13 | 0.77 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 13 | 0.77 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 16 | 0.77 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 7 | 0.77 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 10 | 0.77 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 5 | 0.77 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 4 | 0.76 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 9 | 0.76 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 19 | 0.76 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 1 | 0.76 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 1 | 0.76 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 9 | 0.76 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 9 | 0.76 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 12 | 0.76 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 17 | 0.76 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 16 | 0.76 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 16 | 0.76 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 17 | 0.76 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 17 | 0.76 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 7 | 0.76 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 6 | 0.76 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 6 | 0.76 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 11 | 0.76 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 11 | 0.76 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 20 | 0.76 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 20 | 0.76 |
| (1,423) | 1:A:58:THR:H | 1:A:58:THR:HG23 | 16 | 0.76 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 7 | 0.76 |
| (1,308) | 1:A:41:THR:HG21 | 1:A:53:TRP:HH2 | 16 | 0.76 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 11 | 0.75 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 3 | 0.75 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 12 | 0.75 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 7 | 0.75 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 18 | 0.75 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 18 | 0.75 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 14 | 0.75 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 14 | 0.75 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 15 | 0.75 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 9 | 0.74 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 1 | 0.74 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 1 | 0.74 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 6 | 0.74 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 6 | 0.74 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 19 | 0.74 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 19 | 0.74 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 5 | 0.74 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 3 | 0.74 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 3 | 0.74 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 17 | 0.74 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 17 | 0.74 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 19 | 0.74 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 19 | 0.74 |
| (1,522) | 1:A:73:THR:HG21 | 1:A:74:VAL:H | 3 | 0.74 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 13 | 0.74 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG13 | 17 | 0.74 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG12 | 17 | 0.74 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG13 | 19 | 0.74 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG12 | 19 | 0.74 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 1 | 0.74 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 11 | 0.73 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 18 | 0.73 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 1 | 0.73 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 13 | 0.73 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 5 | 0.73 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 5 | 0.73 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 5 | 0.73 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 12 | 0.73 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 12 | 0.73 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 18 | 0.73 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 18 | 0.73 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 14 | 0.73 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 5 | 0.73 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 8 | 0.73 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 11 | 0.72 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 18 | 0.72 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 17 | 0.72 |
| (1,575) | 1:A:80:GLN:H | 1:A:80:GLN:HB2 | 5 | 0.72 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 7 | 0.72 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 11 | 0.72 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 12 | 0.72 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 20 | 0.72 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 8 | 0.72 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 8 | 0.72 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 15 | 0.72 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 15 | 0.72 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD12 | 3 | 0.72 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD22 | 3 | 0.72 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 20 | 0.72 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,423) | 1:A:58:THR:H | 1:A:58:THR:HG23 | 7 | 0.72 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 12 | 0.72 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 19 | 0.72 |
| (1,377) | 1:A:52:ARG:HB2 | 1:A:75:PHE:HD2 | 2 | 0.72 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 8 | 0.71 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 12 | 0.71 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 20 | 0.71 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 10 | 0.71 |
| (1,535) | 1:A:74:VAL:HG22 | 1:A:81:VAL:HA | 15 | 0.71 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 1 | 0.71 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 1 | 0.71 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 4 | 0.71 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 4 | 0.71 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 7 | 0.71 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 7 | 0.71 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 10 | 0.71 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 10 | 0.71 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 19 | 0.71 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 19 | 0.71 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 19 | 0.71 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 2 | 0.71 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 1 | 0.71 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 1 | 0.71 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 15 | 0.71 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 15 | 0.71 |
| (1,323) | 1:A:44:ILE:HA | 1:A:44:ILE:HD12 | 14 | 0.71 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 6 | 0.71 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 10 | 0.7 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 14 | 0.7 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 3 | 0.7 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 5 | 0.7 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 13 | 0.7 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 6 | 0.69 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 6 | 0.69 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 15 | 0.69 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 15 | 0.69 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 3 | 0.69 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 2 | 0.69 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 2 | 0.69 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 14 | 0.69 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 8 | 0.69 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 10 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,323) | 1:A:44:ILE:HA | 1:A:44:ILE:HD12 | 11 | 0.69 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 2 | 0.69 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 2 | 0.69 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 4 | 0.68 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 11 | 0.68 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 11 | 0.68 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 10 | 0.68 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 9 | 0.68 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 9 | 0.68 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 13 | 0.68 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 19 | 0.68 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 2 | 0.68 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 8 | 0.68 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 12 | 0.68 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 15 | 0.68 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 16 | 0.68 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 20 | 0.68 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 7 | 0.67 |
| (1,486) | 1:A:69:ILE:H | 1:A:69:ILE:HB | 19 | 0.67 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 17 | 0.67 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 3 | 0.67 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 5 | 0.67 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 9 | 0.67 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 11 | 0.67 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 13 | 0.67 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 14 | 0.67 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 18 | 0.67 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 1 | 0.66 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 18 | 0.66 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 1 | 0.66 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 13 | 0.66 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 2 | 0.66 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 12 | 0.66 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 4 | 0.66 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 17 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 1 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 2 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 4 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 6 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 8 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 9 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 10 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 11 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 12 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 13 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 14 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 15 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 16 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 17 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 18 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 19 | 0.66 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 20 | 0.66 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 5 | 0.66 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 6 | 0.65 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 10 | 0.65 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 4 | 0.65 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 16 | 0.65 |
| (1,544) | 1:A:75:PHE:HB2 | 1:A:76:PHE:H | 8 | 0.65 |
| (1,534) | 1:A:74:VAL:HG13 | 1:A:75:PHE:H | 16 | 0.65 |
| (1,534) | 1:A:74:VAL:HG22 | 1:A:75:PHE:H | 16 | 0.65 |
| (1,423) | 1:A:58:THR:H | 1:A:58:THR:HG23 | 10 | 0.65 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 5 | 0.65 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 17 | 0.65 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 17 | 0.65 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 3 | 0.65 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 5 | 0.65 |
| (1,283) | 1:A:38:LEU:HB2 | 1:A:38:LEU:HG | 7 | 0.65 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB3 | 2 | 0.65 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB1 | 2 | 0.65 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB3 | 16 | 0.65 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB1 | 16 | 0.65 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 5 | 0.64 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 2 | 0.64 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 2 | 0.64 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 7 | 0.64 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 7 | 0.64 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 5 | 0.64 |
| (1,645) | 1:A:97:ALA:H | 1:A:97:ALA:HB3 | 4 | 0.64 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 14 | 0.64 |
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 2 | 0.64 |
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 4 | 0.64 |
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 9 | 0.64 |
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 10 | 0.64 |
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 14 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 15 | 0.64 |
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 18 | 0.64 |
| (1,388) | 1:A:53:TRP:H | 1:A:75:PHE:HD2 | 18 | 0.64 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 3 | 0.64 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 3 | 0.64 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 10 | 0.63 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 8 | 0.63 |
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 1 | 0.63 |
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 13 | 0.63 |
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 20 | 0.63 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 9 | 0.63 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 19 | 0.63 |
| (1,388) | 1:A:53:TRP:H | 1:A:75:PHE:HD2 | 11 | 0.63 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 13 | 0.63 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 13 | 0.63 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 18 | 0.63 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 18 | 0.62 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 9 | 0.62 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 5 | 0.62 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 16 | 0.62 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 16 | 0.62 |
| (1,524) | 1:A:73:THR:HG22 | 1:A:75:PHE:HE1 | 10 | 0.62 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 9 | 0.62 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 14 | 0.62 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 18 | 0.62 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 1 | 0.62 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 4 | 0.62 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 17 | 0.62 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 11 | 0.62 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 16 | 0.62 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 4 | 0.62 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 11 | 0.62 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 8 | 0.61 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 19 | 0.61 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 8 | 0.61 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 8 | 0.61 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 4 | 0.61 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 14 | 0.61 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 1 | 0.61 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 4 | 0.61 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 7 | 0.61 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 10 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 11 | 0.61 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 15 | 0.61 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 16 | 0.61 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 17 | 0.61 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD12 | 11 | 0.61 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD22 | 11 | 0.61 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 9 | 0.61 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 20 | 0.61 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG13 | 13 | 0.61 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG12 | 13 | 0.61 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 10 | 0.61 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 3 | 0.61 |
| (1,388) | 1:A:53:TRP:H | 1:A:75:PHE:HD2 | 3 | 0.61 |
| (1,388) | 1:A:53:TRP:H | 1:A:75:PHE:HD2 | 20 | 0.61 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 13 | 0.61 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 14 | 0.61 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 14 | 0.61 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 15 | 0.61 |
| (1,68) | 1:A:15:GLY:H | 1:A:16:ASN:H | 19 | 0.6 |
| (1,653) | 1:A:99:ALA:HA | 1:A:99:ALA:HB2 | 18 | 0.6 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 4 | 0.6 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 4 | 0.6 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 5 | 0.6 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 5 | 0.6 |
| (1,493) | 1:A:69:ILE:HB | 1:A:69:ILE:HG22 | 20 | 0.6 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 1 | 0.6 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 10 | 0.6 |
| (1,388) | 1:A:53:TRP:H | 1:A:75:PHE:HD2 | 12 | 0.6 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 1 | 0.6 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 2 | 0.6 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 6 | 0.6 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 8 | 0.6 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 16 | 0.6 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 17 | 0.6 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 19 | 0.6 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 20 | 0.6 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 15 | 0.6 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 19 | 0.6 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 5 | 0.59 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 20 | 0.59 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 2 | 0.59 |
| (1,646) | 1:A:97:ALA:HA | 1:A:97:ALA:HB2 | 1 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,646) | 1:A:97:ALA:HA | 1:A:97:ALA:HB2 | 8 | 0.59 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 16 | 0.59 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 17 | 0.59 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 20 | 0.59 |
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 2 | 0.59 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 6 | 0.59 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 8 | 0.59 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 12 | 0.59 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 15 | 0.59 |
| (1,436) | 1:A:59:GLN:HA | 1:A:60:ARG:H | 14 | 0.59 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 1 | 0.59 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 11 | 0.59 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 6 | 0.59 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 7 | 0.59 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 11 | 0.59 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 4 | 0.59 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 14 | 0.59 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 9 | 0.59 |
| (1,3) | 1:A:2:ALA:HA | 1:A:2:ALA:HB2 | 15 | 0.59 |
| (1,646) | 1:A:97:ALA:HA | 1:A:97:ALA:HB2 | 16 | 0.58 |
| (1,635) | 1:A:94:GLU:HA | 1:A:95:GLN:H | 3 | 0.58 |
| (1,635) | 1:A:94:GLU:HA | 1:A:95:GLN:H | 12 | 0.58 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 3 | 0.58 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 13 | 0.58 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 14 | 0.58 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 14 | 0.58 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 14 | 0.58 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 14 | 0.58 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 2 | 0.58 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 9 | 0.58 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 4 | 0.58 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 13 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 2 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 5 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 7 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 8 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 9 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 10 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 11 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 12 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 13 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 14 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 15 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 17 | 0.58 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 19 | 0.58 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 15 | 0.58 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 15 | 0.58 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 8 | 0.58 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 19 | 0.57 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 19 | 0.57 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 20 | 0.57 |
| (1,646) | 1:A:97:ALA:HA | 1:A:97:ALA:HB2 | 12 | 0.57 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 2 | 0.57 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 3 | 0.57 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 11 | 0.57 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 18 | 0.57 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 5 | 0.57 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 15 | 0.57 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 18 | 0.57 |
| (1,388) | 1:A:53:TRP:H | 1:A:75:PHE:HD2 | 6 | 0.57 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 4 | 0.57 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 1 | 0.57 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 3 | 0.57 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 10 | 0.57 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 16 | 0.57 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 17 | 0.57 |
| (1,646) | 1:A:97:ALA:HA | 1:A:97:ALA:HB2 | 9 | 0.56 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 13 | 0.56 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 13 | 0.56 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 1 | 0.56 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 5 | 0.56 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 10 | 0.56 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 11 | 0.56 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD12 | 10 | 0.56 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD22 | 10 | 0.56 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 19 | 0.56 |
| (1,448) | 1:A:61:VAL:H | 1:A:62:ASP:H | 11 | 0.56 |
| (1,306) | 1:A:41:THR:HB | 1:A:41:THR:HG21 | 16 | 0.56 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 11 | 0.56 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 7 | 0.56 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 4 | 0.55 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 5 | 0.55 |
| (1,651) | 1:A:99:ALA:H | 1:A:99:ALA:HB2 | 17 | 0.55 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 7 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 7 | 0.55 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 3 | 0.55 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 18 | 0.55 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 4 | 0.55 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 13 | 0.55 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 8 | 0.55 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 13 | 0.55 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 20 | 0.55 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 2 | 0.55 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 16 | 0.54 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 17 | 0.54 |
| (1,700) | 1:A:114:LYS:H | 1:A:115:GLN:H | 1 | 0.54 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 18 | 0.54 |
| (1,626) | 1:A:92:GLN:HA | 1:A:93:ASP:H | 7 | 0.54 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 12 | 0.54 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 5 | 0.54 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 7 | 0.54 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 2 | 0.54 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 7 | 0.54 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 20 | 0.54 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 3 | 0.54 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 3 | 0.54 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 4 | 0.54 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 4 | 0.54 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 14 | 0.54 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 14 | 0.54 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 2 | 0.54 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 7 | 0.54 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 9 | 0.54 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 11 | 0.54 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 9 | 0.54 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 1 | 0.53 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 2 | 0.53 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 20 | 0.53 |
| (1,645) | 1:A:97:ALA:H | 1:A:97:ALA:HB3 | 19 | 0.53 |
| (1,645) | 1:A:97:ALA:H | 1:A:97:ALA:HB3 | 20 | 0.53 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 2 | 0.53 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 16 | 0.53 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 2 | 0.53 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 2 | 0.53 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 8 | 0.53 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 6 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 9 | 0.53 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 20 | 0.53 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 20 | 0.53 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 20 | 0.53 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 20 | 0.53 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 6 | 0.53 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 6 | 0.53 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 6 | 0.53 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 1 | 0.53 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 4 | 0.53 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 5 | 0.53 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 6 | 0.53 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 10 | 0.53 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 12 | 0.53 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 13 | 0.53 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 14 | 0.53 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 17 | 0.53 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 18 | 0.53 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 19 | 0.53 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 16 | 0.53 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 16 | 0.53 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 12 | 0.53 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 12 | 0.52 |
| (1,681) | 1:A:109:ALA:H | 1:A:110:ARG:H | 17 | 0.52 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 7 | 0.52 |
| (1,651) | 1:A:99:ALA:H | 1:A:99:ALA:HB2 | 20 | 0.52 |
| (1,635) | 1:A:94:GLU:HA | 1:A:95:GLN:H | 5 | 0.52 |
| (1,620) | 1:A:91:SER:H | 1:A:92:GLN:H | 8 | 0.52 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 7 | 0.52 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 15 | 0.52 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 10 | 0.52 |
| (1,388) | 1:A:53:TRP:H | 1:A:75:PHE:HD2 | 17 | 0.52 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 15 | 0.52 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 15 | 0.52 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 19 | 0.52 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 19 | 0.52 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 3 | 0.52 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 8 | 0.52 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 15 | 0.52 |
| (1,230) | 1:A:34:GLN:HA | 1:A:34:GLN:HB2 | 16 | 0.52 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 6 | 0.52 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 6 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 9 | 0.51 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 10 | 0.51 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 18 | 0.51 |
| (1,681) | 1:A:109:ALA:H | 1:A:110:ARG:H | 11 | 0.51 |
| (1,681) | 1:A:109:ALA:H | 1:A:110:ARG:H | 19 | 0.51 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 11 | 0.51 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 9 | 0.51 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 9 | 0.51 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 12 | 0.51 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 12 | 0.51 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 9 | 0.51 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 9 | 0.51 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 13 | 0.51 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 7 | 0.51 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 9 | 0.51 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 16 | 0.51 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 15 | 0.51 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 5 | 0.51 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 7 | 0.51 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 8 | 0.51 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 9 | 0.51 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 12 | 0.51 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 16 | 0.51 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 18 | 0.51 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 20 | 0.51 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 5 | 0.51 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 5 | 0.51 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 20 | 0.51 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 20 | 0.51 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 11 | 0.51 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB3 | 18 | 0.51 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB1 | 18 | 0.51 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 16 | 0.5 |
| (1,94) | 1:A:19:LYS:H | 1:A:19:LYS:HA | 16 | 0.5 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 10 | 0.5 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 6 | 0.5 |
| (1,495) | 1:A:69:ILE:HG13 | 1:A:89:PHE:HD2 | 17 | 0.5 |
| (1,479) | 1:A:67:THR:HA | 1:A:67:THR:HG23 | 4 | 0.5 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 9 | 0.5 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 3 | 0.5 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 4 | 0.5 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 6 | 0.5 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 11 | 0.5 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 13 | 0.5 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 15 | 0.5 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 2 | 0.5 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 2 | 0.5 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 13 | 0.5 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 13 | 0.5 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 18 | 0.5 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 18 | 0.5 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 7 | 0.5 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 11 | 0.5 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 19 | 0.5 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 17 | 0.49 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 15 | 0.49 |
| (1,68) | 1:A:15:GLY:H | 1:A:16:ASN:H | 14 | 0.49 |
| (1,661) | 1:A:103:GLN:H | 1:A:104:PHE:H | 6 | 0.49 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 14 | 0.49 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 7 | 0.49 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 7 | 0.49 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 1 | 0.49 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 2 | 0.49 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 10 | 0.49 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 14 | 0.49 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 19 | 0.49 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 12 | 0.49 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 13 | 0.49 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 9 | 0.49 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 9 | 0.49 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 16 | 0.49 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 16 | 0.49 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 17 | 0.49 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 17 | 0.49 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 1 | 0.49 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 2 | 0.49 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 5 | 0.49 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 8 | 0.49 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 9 | 0.49 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 15 | 0.49 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 17 | 0.49 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 18 | 0.49 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 20 | 0.49 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 2 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 6 | 0.48 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 12 | 0.48 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 16 | 0.48 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 7 | 0.48 |
| (1,518) | 1:A:73:THR:HA | 1:A:73:THR:HG21 | 19 | 0.48 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 8 | 0.48 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 8 | 0.48 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 8 | 0.48 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 8 | 0.48 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD12 | 2 | 0.48 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD22 | 2 | 0.48 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD12 | 6 | 0.48 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD22 | 6 | 0.48 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 6 | 0.48 |
| (1,380) | 1:A:52:ARG:HG3 | 1:A:73:THR:HG22 | 10 | 0.48 |
| (1,380) | 1:A:52:ARG:HG3 | 1:A:73:THR:HG22 | 14 | 0.48 |
| (1,356) | 1:A:51:GLN:HA | 1:A:51:GLN:HB2 | 17 | 0.48 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 15 | 0.48 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 1 | 0.48 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 1 | 0.48 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 10 | 0.48 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 10 | 0.48 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 11 | 0.48 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 11 | 0.48 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 12 | 0.48 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 12 | 0.48 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 9 | 0.48 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 9 | 0.48 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 4 | 0.48 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 6 | 0.48 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 10 | 0.48 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 14 | 0.48 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 16 | 0.48 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 6 | 0.48 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 20 | 0.48 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB3 | 10 | 0.48 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB1 | 10 | 0.48 |
| (1,68) | 1:A:15:GLY:H | 1:A:16:ASN:H | 10 | 0.47 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 17 | 0.47 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 1 | 0.47 |
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 20 | 0.47 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 10 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 7 | 0.47 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 7 | 0.47 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 7 | 0.47 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 7 | 0.47 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 3 | 0.47 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 12 | 0.47 |
| (1,162) | 1:A:26:LEU:HB2 | 1:A:26:LEU:HG | 13 | 0.47 |
| (1,99) | 1:A:19:LYS:HA | 1:A:22:ALA:H | 15 | 0.46 |
| (1,420) | 1:A:57:SER:HA | 1:A:58:THR:H | 19 | 0.46 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 19 | 0.46 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 1 | 0.46 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 6 | 0.46 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 19 | 0.46 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 2 | 0.46 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 6 | 0.46 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 20 | 0.46 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG22 | 8 | 0.46 |
| (1,241) | 1:A:35:VAL:HA | 1:A:35:VAL:HG23 | 8 | 0.46 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 8 | 0.45 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 13 | 0.45 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 1 | 0.45 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 9 | 0.45 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 15 | 0.45 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 16 | 0.45 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 5 | 0.45 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 5 | 0.45 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 5 | 0.45 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 8 | 0.45 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 14 | 0.45 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 17 | 0.45 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 2 | 0.45 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 5 | 0.45 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 1 | 0.45 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 4 | 0.45 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 10 | 0.45 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 11 | 0.45 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 12 | 0.45 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 13 | 0.45 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 14 | 0.45 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 15 | 0.45 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 16 | 0.45 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 18 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 19 | 0.45 |
| (1,21) | 1:A:7:ILE:H | 1:A:7:ILE:HB | 8 | 0.45 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 5 | 0.45 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 10 | 0.44 |
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 14 | 0.44 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 4 | 0.44 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 4 | 0.44 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 16 | 0.44 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 11 | 0.44 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 11 | 0.44 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 11 | 0.44 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 15 | 0.44 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 15 | 0.44 |
| (1,523) | 1:A:73:THR:HG21 | 1:A:75:PHE:HD1 | 1 | 0.44 |
| (1,448) | 1:A:61:VAL:H | 1:A:62:ASP:H | 7 | 0.44 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 12 | 0.44 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 15 | 0.44 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 12 | 0.44 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 14 | 0.44 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 10 | 0.44 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 17 | 0.44 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 5 | 0.44 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 7 | 0.44 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 8 | 0.44 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 9 | 0.44 |
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 17 | 0.44 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 14 | 0.43 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 20 | 0.43 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 20 | 0.43 |
| (1,506) | 1:A:71:ASN:H | 1:A:72:PHE:H | 9 | 0.43 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 13 | 0.43 |
| (1,451) | 1:A:61:VAL:HA | 1:A:61:VAL:HG22 | 10 | 0.43 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 13 | 0.43 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 13 | 0.43 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 13 | 0.43 |
| (1,423) | 1:A:58:THR:H | 1:A:58:THR:HG23 | 2 | 0.43 |
| (1,407) | 1:A:56:THR:HA | 1:A:56:THR:HG1 | 19 | 0.43 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 12 | 0.43 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 16 | 0.43 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 14 | 0.43 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 3 | 0.43 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 12 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,288) | 1:A:39:LEU:HA | 1:A:39:LEU:HB2 | 3 | 0.43 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 17 | 0.43 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 11 | 0.42 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 7 | 0.42 |
| (1,647) | 1:A:97:ALA:HA | 1:A:98:LYS:H | 5 | 0.42 |
| (1,630) | 1:A:93:ASP:HA | 1:A:94:GLU:H | 19 | 0.42 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 1 | 0.42 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 1 | 0.42 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 2 | 0.42 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 2 | 0.42 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 12 | 0.42 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 12 | 0.42 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 10 | 0.42 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 10 | 0.42 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 3 | 0.42 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 17 | 0.42 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 8 | 0.42 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 17 | 0.42 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 14 | 0.42 |
| (1,140) | 1:A:23:VAL:HG23 | 1:A:88:TYR:HE1 | 14 | 0.42 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 10 | 0.41 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD12 | 14 | 0.41 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD22 | 14 | 0.41 |
| (1,711) | 1:A:117:GLY:H | 1:A:118:ARG:H | 7 | 0.41 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 4 | 0.41 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 4 | 0.41 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 6 | 0.41 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 6 | 0.41 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 19 | 0.41 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 19 | 0.41 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 18 | 0.41 |
| (1,423) | 1:A:58:THR:H | 1:A:58:THR:HG23 | 12 | 0.41 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 15 | 0.41 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 15 | 0.41 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 16 | 0.41 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 18 | 0.41 |
| (1,138) | 1:A:23:VAL:HG22 | 1:A:24:GLU:H | 14 | 0.41 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 20 | 0.4 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 5 | 0.4 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 12 | 0.4 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD12 | 5 | 0.4 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD22 | 5 | 0.4 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 17 | 0.4 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 17 | 0.4 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 20 | 0.4 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 19 | 0.4 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD12 | 5 | 0.4 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD22 | 5 | 0.4 |
| (1,448) | 1:A:61:VAL:H | 1:A:62:ASP:H | 6 | 0.4 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 12 | 0.4 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 12 | 0.4 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 12 | 0.4 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 5 | 0.4 |
| (1,414) | 1:A:56:THR:HG22 | 1:A:71:ASN:HA | 11 | 0.4 |
| (1,413) | 1:A:56:THR:HG22 | 1:A:69:ILE:HG23 | 18 | 0.4 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 3 | 0.4 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 10 | 0.4 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 20 | 0.4 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 9 | 0.4 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 11 | 0.39 |
| (1,681) | 1:A:109:ALA:H | 1:A:110:ARG:H | 18 | 0.39 |
| (1,68) | 1:A:15:GLY:H | 1:A:16:ASN:H | 3 | 0.39 |
| (1,68) | 1:A:15:GLY:H | 1:A:16:ASN:H | 11 | 0.39 |
| (1,661) | 1:A:103:GLN:H | 1:A:104:PHE:H | 10 | 0.39 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 18 | 0.39 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 11 | 0.39 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 11 | 0.39 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 8 | 0.39 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 8 | 0.39 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 1 | 0.39 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 1 | 0.39 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 1 | 0.39 |
| (1,388) | 1:A:53:TRP:H | 1:A:75:PHE:HD2 | 19 | 0.39 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 13 | 0.39 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 15 | 0.39 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 5 | 0.39 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 6 | 0.39 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 11 | 0.39 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 7 | 0.39 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 11 | 0.39 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 11 | 0.39 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 20 | 0.39 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 20 | 0.39 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 15 | 0.38 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,92) | 1:A:18:ILE:HD12 | 1:A:39:LEU:HD13 | 18 | 0.38 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 9 | 0.38 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 9 | 0.38 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 4 | 0.38 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 10 | 0.38 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 6 | 0.38 |
| (1,665) | 1:A:104:PHE:HA | 1:A:105:GLY:H | 19 | 0.38 |
| (1,627) | 1:A:93:ASP:H | 1:A:93:ASP:HA | 8 | 0.38 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 16 | 0.38 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 16 | 0.38 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG22 | 12 | 0.38 |
| (1,567) | 1:A:77:GLU:H | 1:A:82:VAL:HG23 | 12 | 0.38 |
| (1,432) | 1:A:58:THR:HG22 | 1:A:59:GLN:H | 18 | 0.38 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 18 | 0.38 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 5 | 0.38 |
| (1,696) | 1:A:112:LYS:H | 1:A:113:LYS:H | 13 | 0.37 |
| (1,628) | 1:A:93:ASP:H | 1:A:94:GLU:H | 1 | 0.37 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 10 | 0.37 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD12 | 9 | 0.37 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD22 | 9 | 0.37 |
| (1,456) | 1:A:62:ASP:HA | 1:A:63:ARG:H | 14 | 0.37 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 14 | 0.37 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 9 | 0.37 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 9 | 0.37 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 2 | 0.37 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 18 | 0.37 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 15 | 0.37 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 17 | 0.37 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD12 | 11 | 0.36 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD22 | 11 | 0.36 |
| (1,696) | 1:A:112:LYS:H | 1:A:113:LYS:H | 20 | 0.36 |
| (1,661) | 1:A:103:GLN:H | 1:A:104:PHE:H | 17 | 0.36 |
| (1,651) | 1:A:99:ALA:H | 1:A:99:ALA:HB2 | 11 | 0.36 |
| (1,61) | 1:A:14:GLN:H | 1:A:15:GLY:H | 12 | 0.36 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 19 | 0.36 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 19 | 0.36 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 16 | 0.36 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 5 | 0.36 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 11 | 0.36 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 3 | 0.36 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 4 | 0.36 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 8 | 0.36 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 9 | 0.36 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 17 | 0.36 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 4 | 0.35 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD12 | 19 | 0.35 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD22 | 19 | 0.35 |
| (1,665) | 1:A:104:PHE:HA | 1:A:105:GLY:H | 18 | 0.35 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 17 | 0.35 |
| (1,635) | 1:A:94:GLU:HA | 1:A:95:GLN:H | 13 | 0.35 |
| (1,630) | 1:A:93:ASP:HA | 1:A:94:GLU:H | 11 | 0.35 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 14 | 0.35 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 14 | 0.35 |
| (1,474) | 1:A:66:ARG:H | 1:A:67:THR:H | 10 | 0.35 |
| (1,474) | 1:A:66:ARG:H | 1:A:67:THR:H | 20 | 0.35 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 16 | 0.35 |
| (1,395) | 1:A:54:ASP:HA | 1:A:55:TYR:H | 14 | 0.35 |
| (1,388) | 1:A:53:TRP:H | 1:A:75:PHE:HD2 | 4 | 0.35 |
| (1,357) | 1:A:51:GLN:HA | 1:A:52:ARG:H | 14 | 0.35 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 9 | 0.35 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 10 | 0.35 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 8 | 0.35 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 16 | 0.35 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 2 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 1 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 2 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 6 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 7 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 10 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 11 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 12 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 14 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 15 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 16 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 18 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 19 | 0.35 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 20 | 0.35 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 13 | 0.35 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 16 | 0.35 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 19 | 0.34 |
| (1,678) | 1:A:108:LEU:H | 1:A:109:ALA:H | 20 | 0.34 |
| (1,645) | 1:A:97:ALA:H | 1:A:97:ALA:HB3 | 6 | 0.34 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 3 | 0.34 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 3 | 0.34 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 6 | 0.34 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 6 | 0.34 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 6 | 0.34 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 6 | 0.34 |
| (1,497) | 1:A:69:ILE:HG22 | 1:A:70:LYS:H | 12 | 0.34 |
| (1,486) | 1:A:69:ILE:H | 1:A:69:ILE:HB | 5 | 0.34 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 12 | 0.34 |
| (1,407) | 1:A:56:THR:HA | 1:A:56:THR:HG1 | 14 | 0.34 |
| (1,380) | 1:A:52:ARG:HG3 | 1:A:73:THR:HG22 | 5 | 0.34 |
| (1,380) | 1:A:52:ARG:HG3 | 1:A:73:THR:HG22 | 8 | 0.34 |
| (1,357) | 1:A:51:GLN:HA | 1:A:52:ARG:H | 10 | 0.34 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 4 | 0.34 |
| (1,345) | 1:A:49:HIS:HA | 1:A:49:HIS:HD2 | 15 | 0.34 |
| (1,335) | 1:A:46:ASP:HA | 1:A:48:PHE:H | 19 | 0.34 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 3 | 0.34 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 18 | 0.34 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 10 | 0.34 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 16 | 0.34 |
| (1,18) | 1:A:6:ILE:HA | 1:A:6:ILE:HG22 | 5 | 0.34 |
| (1,111) | 1:A:21:ASN:HA | 1:A:24:GLU:H | 3 | 0.34 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD12 | 1 | 0.33 |
| (1,77) | 1:A:17:LEU:H | 1:A:17:LEU:HD22 | 1 | 0.33 |
| (1,68) | 1:A:15:GLY:H | 1:A:16:ASN:H | 15 | 0.33 |
| (1,665) | 1:A:104:PHE:HA | 1:A:105:GLY:H | 9 | 0.33 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 13 | 0.33 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 6 | 0.33 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG12 | 20 | 0.33 |
| (1,582) | 1:A:81:VAL:H | 1:A:81:VAL:HG22 | 20 | 0.33 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 16 | 0.33 |
| (1,477) | 1:A:67:THR:H | 1:A:67:THR:HB | 6 | 0.33 |
| (1,474) | 1:A:66:ARG:H | 1:A:67:THR:H | 12 | 0.33 |
| (1,413) | 1:A:56:THR:HG22 | 1:A:69:ILE:HG23 | 6 | 0.33 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 20 | 0.33 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 19 | 0.33 |
| (1,345) | 1:A:49:HIS:HA | 1:A:49:HIS:HD2 | 17 | 0.33 |
| (1,336) | 1:A:47:PRO:HA | 1:A:50:ALA:H | 16 | 0.33 |
| (1,301) | 1:A:41:THR:H | 1:A:41:THR:HG22 | 1 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 1 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 2 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 4 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 5 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 6 | 0.33 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 7 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 9 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 10 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 11 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 12 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 13 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 14 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 15 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 16 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 17 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 19 | 0.33 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 20 | 0.33 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 18 | 0.33 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 18 | 0.33 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 4 | 0.33 |
| (1,711) | 1:A:117:GLY:H | 1:A:118:ARG:H | 10 | 0.32 |
| (1,692) | 1:A:111:ASP:HA | 1:A:112:LYS:H | 13 | 0.32 |
| (1,681) | 1:A:109:ALA:H | 1:A:110:ARG:H | 7 | 0.32 |
| (1,663) | 1:A:104:PHE:H | 1:A:105:GLY:H | 6 | 0.32 |
| (1,620) | 1:A:91:SER:H | 1:A:92:GLN:H | 7 | 0.32 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 5 | 0.32 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 15 | 0.32 |
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 8 | 0.32 |
| (1,427) | 1:A:58:THR:HA | 1:A:59:GLN:H | 13 | 0.32 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 9 | 0.32 |
| (1,388) | 1:A:53:TRP:H | 1:A:75:PHE:HD2 | 10 | 0.32 |
| (1,353) | 1:A:50:ALA:HB2 | 1:A:51:GLN:H | 11 | 0.32 |
| (1,335) | 1:A:46:ASP:HA | 1:A:48:PHE:H | 16 | 0.32 |
| (1,335) | 1:A:46:ASP:HA | 1:A:48:PHE:H | 17 | 0.32 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 9 | 0.32 |
| (1,279) | 1:A:38:LEU:HA | 1:A:38:LEU:HB2 | 8 | 0.32 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 8 | 0.32 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 8 | 0.32 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 8 | 0.32 |
| (1,99) | 1:A:19:LYS:HA | 1:A:22:ALA:H | 2 | 0.31 |
| (1,696) | 1:A:112:LYS:H | 1:A:113:LYS:H | 10 | 0.31 |
| (1,665) | 1:A:104:PHE:HA | 1:A:105:GLY:H | 20 | 0.31 |
| (1,663) | 1:A:104:PHE:H | 1:A:105:GLY:H | 1 | 0.31 |
| (1,66) | 1:A:14:GLN:HB2 | 1:A:15:GLY:H | 9 | 0.31 |
| (1,626) | 1:A:92:GLN:HA | 1:A:93:ASP:H | 6 | 0.31 |
| (1,504) | 1:A:70:LYS:HA | 1:A:89:PHE:H | 12 | 0.31 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 14 | 0.31 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 6 | 0.31 |
| (1,448) | 1:A:61:VAL:H | 1:A:62:ASP:H | 16 | 0.31 |
| (1,345) | 1:A:49:HIS:HA | 1:A:49:HIS:HD2 | 7 | 0.31 |
| (1,335) | 1:A:46:ASP:HA | 1:A:48:PHE:H | 14 | 0.31 |
| (1,322) | 1:A:44:ILE:HA | 1:A:44:ILE:HG22 | 4 | 0.31 |
| (1,309) | 1:A:41:THR:HG23 | 1:A:53:TRP:HD1 | 4 | 0.31 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 1 | 0.31 |
| (1,16) | 1:A:6:ILE:H | 1:A:7:ILE:H | 3 | 0.31 |
| (1,705) | 1:A:115:GLN:HA | 1:A:116:ARG:H | 6 | 0.3 |
| (1,635) | 1:A:94:GLU:HA | 1:A:95:GLN:H | 8 | 0.3 |
| (1,630) | 1:A:93:ASP:HA | 1:A:94:GLU:H | 12 | 0.3 |
| (1,512) | 1:A:72:PHE:HA | 1:A:87:ASP:H | 12 | 0.3 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 16 | 0.3 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 7 | 0.3 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 8 | 0.3 |
| (1,335) | 1:A:46:ASP:HA | 1:A:48:PHE:H | 11 | 0.3 |
| (1,99) | 1:A:19:LYS:HA | 1:A:22:ALA:H | 5 | 0.29 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 1 | 0.29 |
| (1,705) | 1:A:115:GLN:HA | 1:A:116:ARG:H | 17 | 0.29 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 9 | 0.29 |
| (1,634) | 1:A:94:GLU:H | 1:A:95:GLN:H | 1 | 0.29 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 20 | 0.29 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 11 | 0.29 |
| (1,48) | 1:A:12:ILE:HA | 1:A:12:ILE:HD12 | 20 | 0.29 |
| (1,477) | 1:A:67:THR:H | 1:A:67:THR:HB | 1 | 0.29 |
| (1,474) | 1:A:66:ARG:H | 1:A:67:THR:H | 15 | 0.29 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 18 | 0.29 |
| (1,194) | 1:A:30:GLN:H | 1:A:81:VAL:H | 5 | 0.29 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 6 | 0.28 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 13 | 0.28 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 1 | 0.28 |
| (1,681) | 1:A:109:ALA:H | 1:A:110:ARG:H | 3 | 0.28 |
| (1,665) | 1:A:104:PHE:HA | 1:A:105:GLY:H | 10 | 0.28 |
| (1,652) | 1:A:99:ALA:H | 1:A:100:ALA:H | 7 | 0.28 |
| (1,626) | 1:A:92:GLN:HA | 1:A:93:ASP:H | 8 | 0.28 |
| (1,477) | 1:A:67:THR:H | 1:A:67:THR:HB | 13 | 0.28 |
| (1,469) | 1:A:64:LEU:HD13 | 1:A:65:ALA:H | 1 | 0.28 |
| (1,431) | 1:A:58:THR:HG1 | 1:A:59:GLN:H | 12 | 0.28 |
| (1,427) | 1:A:58:THR:HA | 1:A:59:GLN:H | 12 | 0.28 |
| (1,380) | 1:A:52:ARG:HG3 | 1:A:73:THR:HG22 | 16 | 0.28 |
| (1,349) | 1:A:50:ALA:H | 1:A:50:ALA:HB2 | 19 | 0.28 |
| (1,12) | 1:A:5:GLY:H | 1:A:6:ILE:H | 5 | 0.28 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 8 | 0.27 |
| (1,704) | 1:A:115:GLN:H | 1:A:116:ARG:H | 4 | 0.27 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 4 | 0.27 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 10 | 0.27 |
| (1,696) | 1:A:112:LYS:H | 1:A:113:LYS:H | 6 | 0.27 |
| (1,696) | 1:A:112:LYS:H | 1:A:113:LYS:H | 19 | 0.27 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 13 | 0.27 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 15 | 0.27 |
| (1,68) | 1:A:15:GLY:H | 1:A:16:ASN:H | 20 | 0.27 |
| (1,634) | 1:A:94:GLU:H | 1:A:95:GLN:H | 4 | 0.27 |
| (1,628) | 1:A:93:ASP:H | 1:A:94:GLU:H | 13 | 0.27 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 19 | 0.27 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 1 | 0.27 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 2 | 0.27 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 6 | 0.27 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 18 | 0.27 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 14 | 0.27 |
| (1,490) | 1:A:69:ILE:HA | 1:A:69:ILE:HG13 | 12 | 0.27 |
| (1,490) | 1:A:69:ILE:HA | 1:A:69:ILE:HG12 | 12 | 0.27 |
| (1,486) | 1:A:69:ILE:H | 1:A:69:ILE:HB | 3 | 0.27 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG13 | 15 | 0.27 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG12 | 15 | 0.27 |
| (1,42) | 1:A:11:PRO:HA | 1:A:12:ILE:H | 17 | 0.27 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 14 | 0.27 |
| (1,406) | 1:A:56:THR:H | 1:A:57:SER:H | 13 | 0.27 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 7 | 0.27 |
| (1,349) | 1:A:50:ALA:H | 1:A:50:ALA:HB2 | 1 | 0.27 |
| (1,349) | 1:A:50:ALA:H | 1:A:50:ALA:HB2 | 6 | 0.27 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 1 | 0.27 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 6 | 0.27 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 6 | 0.27 |
| (1,20) | 1:A:6:ILE:HA | 1:A:8:TYR:H | 19 | 0.27 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 10 | 0.27 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 10 | 0.27 |
| (1,111) | 1:A:21:ASN:HA | 1:A:24:GLU:H | 5 | 0.27 |
| (1,86) | 1:A:18:ILE:HA | 1:A:18:ILE:HD12 | 7 | 0.26 |
| (1,705) | 1:A:115:GLN:HA | 1:A:116:ARG:H | 10 | 0.26 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 14 | 0.26 |
| (1,696) | 1:A:112:LYS:H | 1:A:113:LYS:H | 5 | 0.26 |
| (1,663) | 1:A:104:PHE:H | 1:A:105:GLY:H | 7 | 0.26 |
| (1,634) | 1:A:94:GLU:H | 1:A:95:GLN:H | 6 | 0.26 |
| (1,57) | 1:A:13:TYR:HA | 1:A:14:GLN:H | 12 | 0.26 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 4 | 0.26 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 13 | 0.26 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 14 | 0.26 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 19 | 0.26 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 16 | 0.26 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 10 | 0.26 |
| (1,474) | 1:A:66:ARG:H | 1:A:67:THR:H | 8 | 0.26 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG13 | 9 | 0.26 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG12 | 9 | 0.26 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 5 | 0.26 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 3 | 0.26 |
| (1,335) | 1:A:46:ASP:HA | 1:A:48:PHE:H | 3 | 0.26 |
| (1,273) | 1:A:37:ALA:HA | 1:A:41:THR:H | 6 | 0.26 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 18 | 0.26 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 18 | 0.26 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 4 | 0.26 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 1 | 0.26 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 1 | 0.26 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 12 | 0.25 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 9 | 0.25 |
| (1,93) | 1:A:18:ILE:HD13 | 1:A:88:TYR:HD1 | 8 | 0.25 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 13 | 0.25 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 18 | 0.25 |
| (1,705) | 1:A:115:GLN:HA | 1:A:116:ARG:H | 7 | 0.25 |
| (1,705) | 1:A:115:GLN:HA | 1:A:116:ARG:H | 18 | 0.25 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 2 | 0.25 |
| (1,665) | 1:A:104:PHE:HA | 1:A:105:GLY:H | 5 | 0.25 |
| (1,663) | 1:A:104:PHE:H | 1:A:105:GLY:H | 16 | 0.25 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 14 | 0.25 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 16 | 0.25 |
| (1,57) | 1:A:13:TYR:HA | 1:A:14:GLN:H | 19 | 0.25 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 16 | 0.25 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 3 | 0.25 |
| (1,507) | 1:A:71:ASN:H | 1:A:88:TYR:HA | 15 | 0.25 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 2 | 0.25 |
| (1,473) | 1:A:65:ALA:HB2 | 1:A:66:ARG:H | 10 | 0.25 |
| (1,463) | 1:A:64:LEU:H | 1:A:64:LEU:HG | 6 | 0.25 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 1 | 0.25 |
| (1,413) | 1:A:56:THR:HG22 | 1:A:69:ILE:HG23 | 19 | 0.25 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 2 | 0.25 |
| (1,406) | 1:A:56:THR:H | 1:A:57:SER:H | 14 | 0.25 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 1 | 0.25 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 9 | 0.25 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 5 | 0.25 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 5 | 0.25 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 13 | 0.25 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 13 | 0.25 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 13 | 0.24 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 7 | 0.24 |
| (1,705) | 1:A:115:GLN:HA | 1:A:116:ARG:H | 19 | 0.24 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 8 | 0.24 |
| (1,665) | 1:A:104:PHE:HA | 1:A:105:GLY:H | 11 | 0.24 |
| (1,630) | 1:A:93:ASP:HA | 1:A:94:GLU:H | 20 | 0.24 |
| (1,620) | 1:A:91:SER:H | 1:A:92:GLN:H | 11 | 0.24 |
| (1,604) | 1:A:85:GLU:H | 1:A:86:GLY:H | 12 | 0.24 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 17 | 0.24 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 14 | 0.24 |
| (1,474) | 1:A:66:ARG:H | 1:A:67:THR:H | 14 | 0.24 |
| (1,45) | 1:A:12:ILE:H | 1:A:13:TYR:H | 13 | 0.24 |
| (1,431) | 1:A:58:THR:HG1 | 1:A:59:GLN:H | 18 | 0.24 |
| (1,427) | 1:A:58:THR:HA | 1:A:59:GLN:H | 8 | 0.24 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 13 | 0.24 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 8 | 0.24 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 7 | 0.24 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 20 | 0.24 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 20 | 0.24 |
| (1,349) | 1:A:50:ALA:H | 1:A:50:ALA:HB2 | 7 | 0.24 |
| (1,303) | 1:A:41:THR:HA | 1:A:41:THR:HG1 | 6 | 0.24 |
| (1,30) | 1:A:8:TYR:H | 1:A:9:LYS:H | 3 | 0.24 |
| (1,30) | 1:A:8:TYR:H | 1:A:9:LYS:H | 15 | 0.24 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 1 | 0.24 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 1 | 0.24 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 2 | 0.24 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 2 | 0.24 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 12 | 0.24 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 12 | 0.24 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 12 | 0.24 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 12 | 0.24 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 13 | 0.24 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 13 | 0.24 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 5 | 0.24 |
| (1,169) | 1:A:26:LEU:HD12 | 1:A:84:TRP:HE3 | 13 | 0.24 |
| (1,137) | 1:A:23:VAL:HG12 | 1:A:24:GLU:HA | 14 | 0.24 |
| (1,114) | 1:A:22:ALA:H | 1:A:23:VAL:H | 3 | 0.24 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,99) | 1:A:19:LYS:HA | 1:A:22:ALA:H | 4 | 0.23 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 7 | 0.23 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 16 | 0.23 |
| (1,705) | 1:A:115:GLN:HA | 1:A:116:ARG:H | 9 | 0.23 |
| (1,663) | 1:A:104:PHE:H | 1:A:105:GLY:H | 13 | 0.23 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 15 | 0.23 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 12 | 0.23 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 15 | 0.23 |
| (1,634) | 1:A:94:GLU:H | 1:A:95:GLN:H | 14 | 0.23 |
| (1,628) | 1:A:93:ASP:H | 1:A:94:GLU:H | 5 | 0.23 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 7 | 0.23 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 10 | 0.23 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 11 | 0.23 |
| (1,506) | 1:A:71:ASN:H | 1:A:72:PHE:H | 14 | 0.23 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 3 | 0.23 |
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 10 | 0.23 |
| (1,446) | 1:A:61:VAL:H | 1:A:61:VAL:HB | 16 | 0.23 |
| (1,427) | 1:A:58:THR:HA | 1:A:59:GLN:H | 5 | 0.23 |
| (1,380) | 1:A:52:ARG:HG3 | 1:A:73:THR:HG22 | 17 | 0.23 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 9 | 0.23 |
| (1,345) | 1:A:49:HIS:HA | 1:A:49:HIS:HD2 | 1 | 0.23 |
| (1,331) | 1:A:45:PRO:HA | 1:A:46:ASP:H | 5 | 0.23 |
| (1,32) | 1:A:9:LYS:H | 1:A:10:GLN:HA | 3 | 0.23 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 17 | 0.23 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 17 | 0.23 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 20 | 0.23 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 20 | 0.23 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 17 | 0.23 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 15 | 0.23 |
| (1,700) | 1:A:114:LYS:H | 1:A:115:GLN:H | 19 | 0.22 |
| (1,663) | 1:A:104:PHE:H | 1:A:105:GLY:H | 14 | 0.22 |
| (1,66) | 1:A:14:GLN:HB2 | 1:A:15:GLY:H | 6 | 0.22 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 1 | 0.22 |
| (1,635) | 1:A:94:GLU:HA | 1:A:95:GLN:H | 10 | 0.22 |
| (1,626) | 1:A:92:GLN:HA | 1:A:93:ASP:H | 18 | 0.22 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 9 | 0.22 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 13 | 0.22 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 15 | 0.22 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 5 | 0.22 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 7 | 0.22 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 3 | 0.22 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 13 | 0.22 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 18 | 0.22 |
| (1,486) | 1:A:69:ILE:H | 1:A:69:ILE:HB | 13 | 0.22 |
| (1,474) | 1:A:66:ARG:H | 1:A:67:THR:H | 2 | 0.22 |
| (1,469) | 1:A:64:LEU:HD13 | 1:A:65:ALA:H | 18 | 0.22 |
| (1,456) | 1:A:62:ASP:HA | 1:A:63:ARG:H | 16 | 0.22 |
| (1,434) | 1:A:59:GLN:H | 1:A:68:GLU:H | 10 | 0.22 |
| (1,432) | 1:A:58:THR:HG22 | 1:A:59:GLN:H | 20 | 0.22 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG13 | 10 | 0.22 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG12 | 10 | 0.22 |
| (1,406) | 1:A:56:THR:H | 1:A:57:SER:H | 19 | 0.22 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 4 | 0.22 |
| (1,384) | 1:A:53:TRP:H | 1:A:73:THR:HA | 14 | 0.22 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 2 | 0.22 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 13 | 0.22 |
| (1,32) | 1:A:9:LYS:H | 1:A:10:GLN:HA | 16 | 0.22 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 7 | 0.22 |
| (1,311) | 1:A:42:PRO:HG3 | 1:A:43:SER:H | 9 | 0.22 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 4 | 0.22 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 4 | 0.22 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 7 | 0.22 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 7 | 0.22 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 9 | 0.22 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 9 | 0.22 |
| (1,191) | 1:A:29:GLY:HA2 | 1:A:80:GLN:HB3 | 14 | 0.22 |
| (1,191) | 1:A:29:GLY:HA3 | 1:A:80:GLN:HB3 | 14 | 0.22 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 7 | 0.22 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 5 | 0.22 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 13 | 0.22 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 16 | 0.22 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 18 | 0.22 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 10 | 0.22 |
| (1,15) | 1:A:6:ILE:H | 1:A:6:ILE:HG22 | 13 | 0.22 |
| (1,147) | 1:A:25:GLN:H | 1:A:26:LEU:H | 8 | 0.22 |
| (1,99) | 1:A:19:LYS:HA | 1:A:22:ALA:H | 7 | 0.21 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 15 | 0.21 |
| (1,705) | 1:A:115:GLN:HA | 1:A:116:ARG:H | 12 | 0.21 |
| (1,704) | 1:A:115:GLN:H | 1:A:116:ARG:H | 15 | 0.21 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 12 | 0.21 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 9 | 0.21 |
| (1,692) | 1:A:111:ASP:HA | 1:A:112:LYS:H | 1 | 0.21 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 4 | 0.21 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 19 | 0.21 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,628) | 1:A:93:ASP:H | 1:A:94:GLU:H | 10 | 0.21 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 5 | 0.21 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 16 | 0.21 |
| (1,524) | 1:A:73:THR:HG22 | 1:A:75:PHE:HE1 | 19 | 0.21 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 15 | 0.21 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 17 | 0.21 |
| (1,512) | 1:A:72:PHE:HA | 1:A:87:ASP:H | 9 | 0.21 |
| (1,506) | 1:A:71:ASN:H | 1:A:72:PHE:H | 16 | 0.21 |
| (1,490) | 1:A:69:ILE:HA | 1:A:69:ILE:HG13 | 19 | 0.21 |
| (1,490) | 1:A:69:ILE:HA | 1:A:69:ILE:HG12 | 19 | 0.21 |
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 14 | 0.21 |
| (1,432) | 1:A:58:THR:HG22 | 1:A:59:GLN:H | 9 | 0.21 |
| (1,42) | 1:A:11:PRO:HA | 1:A:12:ILE:H | 3 | 0.21 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 10 | 0.21 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 3 | 0.21 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 3 | 0.21 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 12 | 0.21 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 14 | 0.21 |
| (1,331) | 1:A:45:PRO:HA | 1:A:46:ASP:H | 6 | 0.21 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 13 | 0.21 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 15 | 0.21 |
| (1,250) | 1:A:35:VAL:HG11 | 1:A:39:LEU:HD11 | 1 | 0.21 |
| (1,250) | 1:A:35:VAL:HG11 | 1:A:39:LEU:HD11 | 17 | 0.21 |
| (1,221) | 1:A:33:GLN:HA | 1:A:37:ALA:H | 16 | 0.21 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 11 | 0.21 |
| (1,20) | 1:A:6:ILE:HA | 1:A:8:TYR:H | 11 | 0.21 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 19 | 0.21 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 2 | 0.21 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 9 | 0.21 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 10 | 0.21 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 14 | 0.21 |
| (1,165) | 1:A:26:LEU:HB2 | 1:A:84:TRP:HZ2 | 19 | 0.21 |
| (1,135) | 1:A:23:VAL:HG11 | 1:A:84:TRP:HD1 | 5 | 0.21 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 14 | 0.2 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 18 | 0.2 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 13 | 0.2 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 6 | 0.2 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 2 | 0.2 |
| (1,663) | 1:A:104:PHE:H | 1:A:105:GLY:H | 15 | 0.2 |
| (1,652) | 1:A:99:ALA:H | 1:A:100:ALA:H | 8 | 0.2 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 14 | 0.2 |
| (1,631) | 1:A:93:ASP:HA | 1:A:95:GLN:H | 16 | 0.2 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,628) | 1:A:93:ASP:H | 1:A:94:GLU:H | 8 | 0.2 |
| (1,626) | 1:A:92:GLN:HA | 1:A:93:ASP:H | 10 | 0.2 |
| (1,604) | 1:A:85:GLU:H | 1:A:86:GLY:H | 8 | 0.2 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 8 | 0.2 |
| (1,597) | 1:A:83:ARG:HA | 1:A:84:TRP:H | 4 | 0.2 |
| (1,594) | 1:A:83:ARG:H | 1:A:83:ARG:HE | 18 | 0.2 |
| (1,58) | 1:A:14:GLN:H | 1:A:14:GLN:HA | 12 | 0.2 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 10 | 0.2 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 10 | 0.2 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 10 | 0.2 |
| (1,477) | 1:A:67:THR:H | 1:A:67:THR:HB | 9 | 0.2 |
| (1,477) | 1:A:67:THR:H | 1:A:67:THR:HB | 10 | 0.2 |
| (1,470) | 1:A:65:ALA:H | 1:A:65:ALA:HB2 | 17 | 0.2 |
| (1,470) | 1:A:65:ALA:H | 1:A:65:ALA:HB3 | 17 | 0.2 |
| (1,463) | 1:A:64:LEU:H | 1:A:64:LEU:HG | 4 | 0.2 |
| (1,431) | 1:A:58:THR:HG1 | 1:A:59:GLN:H | 14 | 0.2 |
| (1,42) | 1:A:11:PRO:HA | 1:A:12:ILE:H | 8 | 0.2 |
| (1,403) | 1:A:55:TYR:H | 1:A:73:THR:HA | 8 | 0.2 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 15 | 0.2 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 7 | 0.2 |
| (1,335) | 1:A:46:ASP:HA | 1:A:48:PHE:H | 6 | 0.2 |
| (1,32) | 1:A:9:LYS:H | 1:A:10:GLN:HA | 15 | 0.2 |
| (1,30) | 1:A:8:TYR:H | 1:A:9:LYS:H | 8 | 0.2 |
| (1,293) | 1:A:39:LEU:HD12 | 1:A:53:TRP:HH2 | 18 | 0.2 |
| (1,193) | 1:A:30:GLN:H | 1:A:31:SER:H | 12 | 0.2 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 9 | 0.2 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 7 | 0.2 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 12 | 0.2 |
| (1,169) | 1:A:26:LEU:HD12 | 1:A:84:TRP:HE3 | 14 | 0.2 |
| (1,109) | 1:A:21:ASN:H | 1:A:23:VAL:H | 1 | 0.2 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 2 | 0.19 |
| (1,95) | 1:A:19:LYS:H | 1:A:20:GLN:H | 17 | 0.19 |
| (1,85) | 1:A:18:ILE:HA | 1:A:18:ILE:HG22 | 1 | 0.19 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 3 | 0.19 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 16 | 0.19 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 7 | 0.19 |
| (1,639) | 1:A:95:GLN:HA | 1:A:96:LEU:H | 10 | 0.19 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 18 | 0.19 |
| (1,634) | 1:A:94:GLU:H | 1:A:95:GLN:H | 18 | 0.19 |
| (1,628) | 1:A:93:ASP:H | 1:A:94:GLU:H | 9 | 0.19 |
| (1,620) | 1:A:91:SER:H | 1:A:92:GLN:H | 10 | 0.19 |
| (1,597) | 1:A:83:ARG:HA | 1:A:84:TRP:H | 10 | 0.19 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,58) | 1:A:14:GLN:H | 1:A:14:GLN:HA | 19 | 0.19 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 1 | 0.19 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 8 | 0.19 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 1 | 0.19 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 3 | 0.19 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 6 | 0.19 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 12 | 0.19 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 13 | 0.19 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 18 | 0.19 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 20 | 0.19 |
| (1,507) | 1:A:71:ASN:H | 1:A:88:TYR:HA | 10 | 0.19 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 8 | 0.19 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 15 | 0.19 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 2 | 0.19 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 10 | 0.19 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD12 | 1 | 0.19 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD22 | 1 | 0.19 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 4 | 0.19 |
| (1,412) | 1:A:56:THR:HG21 | 1:A:71:ASN:HA | 5 | 0.19 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 4 | 0.19 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 17 | 0.19 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 12 | 0.19 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 12 | 0.19 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 10 | 0.19 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 7 | 0.19 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 3 | 0.19 |
| (1,273) | 1:A:37:ALA:HA | 1:A:41:THR:H | 16 | 0.19 |
| (1,263) | 1:A:36:SER:HA | 1:A:40:GLY:H | 6 | 0.19 |
| (1,250) | 1:A:35:VAL:HG11 | 1:A:39:LEU:HD11 | 18 | 0.19 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 14 | 0.19 |
| (1,203) | 1:A:31:SER:HA | 1:A:34:GLN:H | 3 | 0.19 |
| (1,2) | 1:A:2:ALA:H | 1:A:3:GLY:H | 12 | 0.19 |
| (1,193) | 1:A:30:GLN:H | 1:A:31:SER:H | 7 | 0.19 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 6 | 0.19 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 17 | 0.19 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 20 | 0.19 |
| (1,169) | 1:A:26:LEU:HD12 | 1:A:84:TRP:HE3 | 1 | 0.19 |
| (1,16) | 1:A:6:ILE:H | 1:A:7:ILE:H | 6 | 0.19 |
| (1,137) | 1:A:23:VAL:HG12 | 1:A:24:GLU:HA | 8 | 0.19 |
| (1,135) | 1:A:23:VAL:HG11 | 1:A:84:TRP:HD1 | 7 | 0.19 |
| (1,132) | 1:A:23:VAL:HB | 1:A:24:GLU:H | 3 | 0.19 |
| (1,111) | 1:A:21:ASN:HA | 1:A:24:GLU:H | 1 | 0.19 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,101) | 1:A:20:GLN:H | 1:A:20:GLN:HA | 1 | 0.19 |
| (1,101) | 1:A:20:GLN:H | 1:A:20:GLN:HA | 11 | 0.19 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 20 | 0.18 |
| (1,85) | 1:A:18:ILE:HA | 1:A:18:ILE:HG22 | 12 | 0.18 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 11 | 0.18 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 2 | 0.18 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 10 | 0.18 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 11 | 0.18 |
| (1,696) | 1:A:112:LYS:H | 1:A:113:LYS:H | 15 | 0.18 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 1 | 0.18 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 17 | 0.18 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 18 | 0.18 |
| (1,679) | 1:A:108:LEU:HA | 1:A:109:ALA:H | 6 | 0.18 |
| (1,65) | 1:A:14:GLN:HA | 1:A:16:ASN:H | 1 | 0.18 |
| (1,644) | 1:A:97:ALA:H | 1:A:97:ALA:HA | 5 | 0.18 |
| (1,644) | 1:A:97:ALA:H | 1:A:97:ALA:HA | 6 | 0.18 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 5 | 0.18 |
| (1,622) | 1:A:91:SER:HA | 1:A:92:GLN:H | 4 | 0.18 |
| (1,604) | 1:A:85:GLU:H | 1:A:86:GLY:H | 15 | 0.18 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 13 | 0.18 |
| (1,521) | 1:A:73:THR:HG1 | 1:A:74:VAL:H | 1 | 0.18 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 1 | 0.18 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 3 | 0.18 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 3 | 0.18 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB3 | 3 | 0.18 |
| (1,508) | 1:A:71:ASN:H | 1:A:88:TYR:HB2 | 3 | 0.18 |
| (1,506) | 1:A:71:ASN:H | 1:A:72:PHE:H | 18 | 0.18 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 16 | 0.18 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 18 | 0.18 |
| (1,487) | 1:A:69:ILE:H | 1:A:69:ILE:HG12 | 7 | 0.18 |
| (1,485) | 1:A:68:GLU:HA | 1:A:69:ILE:H | 13 | 0.18 |
| (1,474) | 1:A:66:ARG:H | 1:A:67:THR:H | 3 | 0.18 |
| (1,45) | 1:A:12:ILE:H | 1:A:13:TYR:H | 9 | 0.18 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 16 | 0.18 |
| (1,432) | 1:A:58:THR:HG22 | 1:A:59:GLN:H | 6 | 0.18 |
| (1,431) | 1:A:58:THR:HG1 | 1:A:59:GLN:H | 6 | 0.18 |
| (1,428) | 1:A:58:THR:HB | 1:A:59:GLN:H | 18 | 0.18 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 17 | 0.18 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 20 | 0.18 |
| (1,357) | 1:A:51:GLN:HA | 1:A:52:ARG:H | 2 | 0.18 |
| (1,32) | 1:A:9:LYS:H | 1:A:10:GLN:HA | 17 | 0.18 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 1 | 0.18 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 3 | 0.18 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 18 | 0.18 |
| (1,273) | 1:A:37:ALA:HA | 1:A:41:THR:H | 20 | 0.18 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 11 | 0.18 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 11 | 0.18 |
| (1,227) | 1:A:34:GLN:H | 1:A:35:VAL:H | 8 | 0.18 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 4 | 0.18 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 3 | 0.18 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 11 | 0.18 |
| (1,175) | 1:A:27:GLN:H | 1:A:28:VAL:H | 14 | 0.18 |
| (1,168) | 1:A:26:LEU:HD12 | 1:A:84:TRP:HD1 | 14 | 0.18 |
| (1,136) | 1:A:23:VAL:HG12 | 1:A:24:GLU:H | 1 | 0.18 |
| (1,136) | 1:A:23:VAL:HG12 | 1:A:24:GLU:H | 5 | 0.18 |
| (1,12) | 1:A:5:GLY:H | 1:A:6:ILE:H | 17 | 0.18 |
| (1,114) | 1:A:22:ALA:H | 1:A:23:VAL:H | 5 | 0.18 |
| (1,74) | 1:A:16:ASN:HA | 1:A:18:ILE:H | 18 | 0.17 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 9 | 0.17 |
| (1,705) | 1:A:115:GLN:HA | 1:A:116:ARG:H | 16 | 0.17 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 1 | 0.17 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 17 | 0.17 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 20 | 0.17 |
| (1,678) | 1:A:108:LEU:H | 1:A:109:ALA:H | 1 | 0.17 |
| (1,652) | 1:A:99:ALA:H | 1:A:100:ALA:H | 14 | 0.17 |
| (1,648) | 1:A:98:LYS:HA | 1:A:99:ALA:H | 12 | 0.17 |
| (1,630) | 1:A:93:ASP:HA | 1:A:94:GLU:H | 17 | 0.17 |
| (1,628) | 1:A:93:ASP:H | 1:A:94:GLU:H | 7 | 0.17 |
| (1,626) | 1:A:92:GLN:HA | 1:A:93:ASP:H | 13 | 0.17 |
| (1,623) | 1:A:92:GLN:H | 1:A:93:ASP:H | 3 | 0.17 |
| (1,622) | 1:A:91:SER:HA | 1:A:92:GLN:H | 14 | 0.17 |
| (1,62) | 1:A:14:GLN:HA | 1:A:14:GLN:HB2 | 15 | 0.17 |
| (1,618) | 1:A:90:PRO:HA | 1:A:91:SER:H | 9 | 0.17 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 4 | 0.17 |
| (1,597) | 1:A:83:ARG:HA | 1:A:84:TRP:H | 1 | 0.17 |
| (1,597) | 1:A:83:ARG:HA | 1:A:84:TRP:H | 9 | 0.17 |
| (1,58) | 1:A:14:GLN:H | 1:A:14:GLN:HA | 9 | 0.17 |
| (1,566) | 1:A:77:GLU:H | 1:A:81:VAL:HA | 7 | 0.17 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 20 | 0.17 |
| (1,555) | 1:A:76:PHE:HA | 1:A:82:VAL:H | 18 | 0.17 |
| (1,552) | 1:A:76:PHE:HA | 1:A:78:ASN:H | 8 | 0.17 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 13 | 0.17 |
| (1,521) | 1:A:73:THR:HG1 | 1:A:74:VAL:H | 19 | 0.17 |
| (1,507) | 1:A:71:ASN:H | 1:A:88:TYR:HA | 7 | 0.17 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,506) | 1:A:71:ASN:H | 1:A:72:PHE:H | 3 | 0.17 |
| (1,490) | 1:A:69:ILE:HA | 1:A:69:ILE:HG13 | 5 | 0.17 |
| (1,490) | 1:A:69:ILE:HA | 1:A:69:ILE:HG12 | 5 | 0.17 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 9 | 0.17 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 17 | 0.17 |
| (1,483) | 1:A:68:GLU:H | 1:A:69:ILE:H | 2 | 0.17 |
| (1,483) | 1:A:68:GLU:H | 1:A:69:ILE:H | 6 | 0.17 |
| (1,483) | 1:A:68:GLU:H | 1:A:69:ILE:H | 16 | 0.17 |
| (1,473) | 1:A:65:ALA:HB2 | 1:A:66:ARG:H | 2 | 0.17 |
| (1,45) | 1:A:12:ILE:H | 1:A:13:TYR:H | 15 | 0.17 |
| (1,441) | 1:A:60:ARG:HA | 1:A:61:VAL:H | 1 | 0.17 |
| (1,441) | 1:A:60:ARG:HA | 1:A:61:VAL:H | 14 | 0.17 |
| (1,432) | 1:A:58:THR:HG22 | 1:A:59:GLN:H | 1 | 0.17 |
| (1,421) | 1:A:57:SER:HA | 1:A:58:THR:HB | 18 | 0.17 |
| (1,417) | 1:A:57:SER:H | 1:A:71:ASN:H | 20 | 0.17 |
| (1,407) | 1:A:56:THR:HA | 1:A:56:THR:HG1 | 3 | 0.17 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 3 | 0.17 |
| (1,396) | 1:A:54:ASP:HA | 1:A:73:THR:HA | 16 | 0.17 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 19 | 0.17 |
| (1,384) | 1:A:53:TRP:H | 1:A:73:THR:HA | 8 | 0.17 |
| (1,382) | 1:A:52:ARG:HG2 | 1:A:73:THR:HG22 | 13 | 0.17 |
| (1,380) | 1:A:52:ARG:HG3 | 1:A:73:THR:HG22 | 4 | 0.17 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 8 | 0.17 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG21 | 19 | 0.17 |
| (1,371) | 1:A:52:ARG:HB3 | 1:A:73:THR:HG22 | 19 | 0.17 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 8 | 0.17 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 11 | 0.17 |
| (1,358) | 1:A:51:GLN:HB3 | 1:A:52:ARG:H | 14 | 0.17 |
| (1,32) | 1:A:9:LYS:H | 1:A:10:GLN:HA | 1 | 0.17 |
| (1,250) | 1:A:35:VAL:HG11 | 1:A:39:LEU:HD11 | 12 | 0.17 |
| (1,250) | 1:A:35:VAL:HG11 | 1:A:39:LEU:HD11 | 19 | 0.17 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 10 | 0.17 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 10 | 0.17 |
| (1,193) | 1:A:30:GLN:H | 1:A:31:SER:H | 4 | 0.17 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 1 | 0.17 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 3 | 0.17 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 1 | 0.17 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 8 | 0.17 |
| (1,152) | 1:A:26:LEU:H | 1:A:26:LEU:HA | 8 | 0.17 |
| (1,136) | 1:A:23:VAL:HG12 | 1:A:24:GLU:H | 19 | 0.17 |
| (1,135) | 1:A:23:VAL:HG11 | 1:A:84:TRP:HD1 | 1 | 0.17 |
| (1,120) | 1:A:22:ALA:HA | 1:A:26:LEU:H | 16 | 0.17 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,113) | 1:A:21:ASN:HA | 1:A:25:GLN:H | 11 | 0.17 |
| (1,111) | 1:A:21:ASN:HA | 1:A:24:GLU:H | 7 | 0.17 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 13 | 0.16 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD23 | 17 | 0.16 |
| (1,89) | 1:A:18:ILE:HA | 1:A:39:LEU:HD21 | 17 | 0.16 |
| (1,700) | 1:A:114:LYS:H | 1:A:115:GLN:H | 12 | 0.16 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 6 | 0.16 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 8 | 0.16 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 17 | 0.16 |
| (1,663) | 1:A:104:PHE:H | 1:A:105:GLY:H | 10 | 0.16 |
| (1,651) | 1:A:99:ALA:H | 1:A:99:ALA:HB2 | 12 | 0.16 |
| (1,65) | 1:A:14:GLN:HA | 1:A:16:ASN:H | 9 | 0.16 |
| (1,640) | 1:A:96:LEU:H | 1:A:96:LEU:HA | 1 | 0.16 |
| (1,640) | 1:A:96:LEU:H | 1:A:96:LEU:HA | 2 | 0.16 |
| (1,640) | 1:A:96:LEU:H | 1:A:96:LEU:HA | 11 | 0.16 |
| (1,628) | 1:A:93:ASP:H | 1:A:94:GLU:H | 4 | 0.16 |
| (1,628) | 1:A:93:ASP:H | 1:A:94:GLU:H | 14 | 0.16 |
| (1,620) | 1:A:91:SER:H | 1:A:92:GLN:H | 19 | 0.16 |
| (1,618) | 1:A:90:PRO:HA | 1:A:91:SER:H | 5 | 0.16 |
| (1,604) | 1:A:85:GLU:H | 1:A:86:GLY:H | 6 | 0.16 |
| (1,554) | 1:A:76:PHE:HA | 1:A:81:VAL:HA | 7 | 0.16 |
| (1,552) | 1:A:76:PHE:HA | 1:A:78:ASN:H | 17 | 0.16 |
| (1,532) | 1:A:74:VAL:HB | 1:A:85:GLU:H | 19 | 0.16 |
| (1,521) | 1:A:73:THR:HG1 | 1:A:74:VAL:H | 17 | 0.16 |
| (1,507) | 1:A:71:ASN:H | 1:A:88:TYR:HA | 4 | 0.16 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 7 | 0.16 |
| (1,497) | 1:A:69:ILE:HG22 | 1:A:70:LYS:H | 5 | 0.16 |
| (1,474) | 1:A:66:ARG:H | 1:A:67:THR:H | 18 | 0.16 |
| (1,473) | 1:A:65:ALA:HB2 | 1:A:66:ARG:H | 13 | 0.16 |
| (1,449) | 1:A:61:VAL:H | 1:A:67:THR:HA | 14 | 0.16 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 4 | 0.16 |
| (1,439) | 1:A:60:ARG:H | 1:A:61:VAL:H | 17 | 0.16 |
| (1,431) | 1:A:58:THR:HG1 | 1:A:59:GLN:H | 13 | 0.16 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 8 | 0.16 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 8 | 0.16 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 8 | 0.16 |
| (1,424) | 1:A:58:THR:H | 1:A:59:GLN:H | 5 | 0.16 |
| (1,403) | 1:A:55:TYR:H | 1:A:73:THR:HA | 13 | 0.16 |
| (1,395) | 1:A:54:ASP:HA | 1:A:55:TYR:H | 13 | 0.16 |
| (1,384) | 1:A:53:TRP:H | 1:A:73:THR:HA | 10 | 0.16 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 3 | 0.16 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 10 | 0.16 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 1 | 0.16 |
| (1,345) | 1:A:49:HIS:HA | 1:A:49:HIS:HD2 | 3 | 0.16 |
| (1,300) | 1:A:41:THR:H | 1:A:41:THR:HG1 | 3 | 0.16 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 16 | 0.16 |
| (1,273) | 1:A:37:ALA:HA | 1:A:41:THR:H | 15 | 0.16 |
| (1,228) | 1:A:34:GLN:H | 1:A:36:SER:H | 6 | 0.16 |
| (1,220) | 1:A:33:GLN:HA | 1:A:36:SER:H | 9 | 0.16 |
| (1,208) | 1:A:32:LYS:H | 1:A:33:GLN:H | 12 | 0.16 |
| (1,2) | 1:A:2:ALA:H | 1:A:3:GLY:H | 5 | 0.16 |
| (1,19) | 1:A:6:ILE:HA | 1:A:7:ILE:H | 8 | 0.16 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 16 | 0.16 |
| (1,175) | 1:A:27:GLN:H | 1:A:28:VAL:H | 19 | 0.16 |
| (1,161) | 1:A:26:LEU:HA | 1:A:28:VAL:H | 7 | 0.16 |
| (1,147) | 1:A:25:GLN:H | 1:A:26:LEU:H | 6 | 0.16 |
| (1,137) | 1:A:23:VAL:HG12 | 1:A:24:GLU:HA | 18 | 0.16 |
| (1,136) | 1:A:23:VAL:HG12 | 1:A:24:GLU:H | 4 | 0.16 |
| (1,136) | 1:A:23:VAL:HG12 | 1:A:24:GLU:H | 8 | 0.16 |
| (1,135) | 1:A:23:VAL:HG11 | 1:A:84:TRP:HD1 | 9 | 0.16 |
| (1,110) | 1:A:21:ASN:H | 1:A:24:GLU:H | 1 | 0.16 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB3 | 6 | 0.16 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB1 | 6 | 0.16 |
| (1,98) | 1:A:19:LYS:HA | 1:A:21:ASN:H | 4 | 0.15 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 8 | 0.15 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 9 | 0.15 |
| (1,700) | 1:A:114:LYS:H | 1:A:115:GLN:H | 9 | 0.15 |
| (1,700) | 1:A:114:LYS:H | 1:A:115:GLN:H | 16 | 0.15 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 18 | 0.15 |
| (1,699) | 1:A:113:LYS:HA | 1:A:114:LYS:H | 15 | 0.15 |
| (1,697) | 1:A:112:LYS:HA | 1:A:113:LYS:H | 1 | 0.15 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 16 | 0.15 |
| (1,678) | 1:A:108:LEU:H | 1:A:109:ALA:H | 17 | 0.15 |
| (1,676) | 1:A:108:LEU:H | 1:A:108:LEU:HA | 6 | 0.15 |
| (1,676) | 1:A:108:LEU:H | 1:A:108:LEU:HA | 17 | 0.15 |
| (1,64) | 1:A:14:GLN:HA | 1:A:15:GLY:H | 2 | 0.15 |
| (1,632) | 1:A:94:GLU:H | 1:A:94:GLU:HA | 7 | 0.15 |
| (1,632) | 1:A:94:GLU:H | 1:A:94:GLU:HA | 17 | 0.15 |
| (1,626) | 1:A:92:GLN:HA | 1:A:93:ASP:H | 2 | 0.15 |
| (1,623) | 1:A:92:GLN:H | 1:A:93:ASP:H | 19 | 0.15 |
| (1,597) | 1:A:83:ARG:HA | 1:A:84:TRP:H | 7 | 0.15 |
| (1,594) | 1:A:83:ARG:H | 1:A:83:ARG:HE | 3 | 0.15 |
| (1,594) | 1:A:83:ARG:H | 1:A:83:ARG:HE | 19 | 0.15 |
| (1,588) | 1:A:82:VAL:H | 1:A:83:ARG:H | 4 | 0.15 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 11 | 0.15 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 12 | 0.15 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 6 | 0.15 |
| (1,55) | 1:A:13:TYR:H | 1:A:14:GLN:H | 13 | 0.15 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 14 | 0.15 |
| (1,536) | 1:A:74:VAL:HG21 | 1:A:84:TRP:HZ3 | 10 | 0.15 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 9 | 0.15 |
| (1,521) | 1:A:73:THR:HG1 | 1:A:74:VAL:H | 18 | 0.15 |
| (1,52) | 1:A:12:ILE:HG23 | 1:A:13:TYR:H | 2 | 0.15 |
| (1,506) | 1:A:71:ASN:H | 1:A:72:PHE:H | 12 | 0.15 |
| (1,506) | 1:A:71:ASN:H | 1:A:72:PHE:H | 15 | 0.15 |
| (1,503) | 1:A:70:LYS:HA | 1:A:88:TYR:HA | 16 | 0.15 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 20 | 0.15 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 15 | 0.15 |
| (1,483) | 1:A:68:GLU:H | 1:A:69:ILE:H | 9 | 0.15 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 15 | 0.15 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 19 | 0.15 |
| (1,439) | 1:A:60:ARG:H | 1:A:61:VAL:H | 11 | 0.15 |
| (1,431) | 1:A:58:THR:HG1 | 1:A:59:GLN:H | 8 | 0.15 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG13 | 1 | 0.15 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG12 | 1 | 0.15 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG13 | 14 | 0.15 |
| (1,429) | 1:A:58:THR:HB | 1:A:69:ILE:HG12 | 14 | 0.15 |
| (1,424) | 1:A:58:THR:H | 1:A:59:GLN:H | 12 | 0.15 |
| (1,403) | 1:A:55:TYR:H | 1:A:73:THR:HA | 2 | 0.15 |
| (1,402) | 1:A:55:TYR:H | 1:A:56:THR:H | 14 | 0.15 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 2 | 0.15 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 17 | 0.15 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 12 | 0.15 |
| (1,357) | 1:A:51:GLN:HA | 1:A:52:ARG:H | 20 | 0.15 |
| (1,351) | 1:A:50:ALA:HA | 1:A:50:ALA:HB2 | 7 | 0.15 |
| (1,335) | 1:A:46:ASP:HA | 1:A:48:PHE:H | 4 | 0.15 |
| (1,323) | 1:A:44:ILE:HA | 1:A:44:ILE:HD12 | 9 | 0.15 |
| (1,32) | 1:A:9:LYS:H | 1:A:10:GLN:HA | 10 | 0.15 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 15 | 0.15 |
| (1,312) | 1:A:43:SER:H | 1:A:43:SER:HA | 18 | 0.15 |
| (1,30) | 1:A:8:TYR:H | 1:A:9:LYS:H | 16 | 0.15 |
| (1,30) | 1:A:8:TYR:H | 1:A:9:LYS:H | 18 | 0.15 |
| (1,293) | 1:A:39:LEU:HD12 | 1:A:53:TRP:HH2 | 11 | 0.15 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 1 | 0.15 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 5 | 0.15 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 11 | 0.15 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 17 | 0.15 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 19 | 0.15 |
| (1,28) | 1:A:8:TYR:H | 1:A:8:TYR:HA | 14 | 0.15 |
| (1,264) | 1:A:36:SER:HA | 1:A:53:TRP:HZ2 | 16 | 0.15 |
| (1,250) | 1:A:35:VAL:HG11 | 1:A:39:LEU:HD11 | 3 | 0.15 |
| (1,249) | 1:A:35:VAL:HB | 1:A:76:PHE:HE1 | 5 | 0.15 |
| (1,221) | 1:A:33:GLN:HA | 1:A:37:ALA:H | 6 | 0.15 |
| (1,211) | 1:A:32:LYS:HA | 1:A:35:VAL:H | 18 | 0.15 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 2 | 0.15 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 6 | 0.15 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 20 | 0.15 |
| (1,169) | 1:A:26:LEU:HD12 | 1:A:84:TRP:HE3 | 5 | 0.15 |
| (1,169) | 1:A:26:LEU:HD12 | 1:A:84:TRP:HE3 | 7 | 0.15 |
| (1,147) | 1:A:25:GLN:H | 1:A:26:LEU:H | 11 | 0.15 |
| (1,137) | 1:A:23:VAL:HG12 | 1:A:24:GLU:HA | 16 | 0.15 |
| (1,136) | 1:A:23:VAL:HG12 | 1:A:24:GLU:H | 3 | 0.15 |
| (1,101) | 1:A:20:GLN:H | 1:A:20:GLN:HA | 12 | 0.15 |
| (1,83) | 1:A:18:ILE:H | 1:A:18:ILE:HD12 | 1 | 0.14 |
| (1,80) | 1:A:18:ILE:H | 1:A:18:ILE:HB | 14 | 0.14 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 2 | 0.14 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 11 | 0.14 |
| (1,704) | 1:A:115:GLN:H | 1:A:116:ARG:H | 14 | 0.14 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 20 | 0.14 |
| (1,699) | 1:A:113:LYS:HA | 1:A:114:LYS:H | 17 | 0.14 |
| (1,696) | 1:A:112:LYS:H | 1:A:113:LYS:H | 3 | 0.14 |
| (1,694) | 1:A:112:LYS:H | 1:A:112:LYS:HA | 5 | 0.14 |
| (1,692) | 1:A:111:ASP:HA | 1:A:112:LYS:H | 3 | 0.14 |
| (1,685) | 1:A:110:ARG:H | 1:A:111:ASP:H | 1 | 0.14 |
| (1,685) | 1:A:110:ARG:H | 1:A:111:ASP:H | 17 | 0.14 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 9 | 0.14 |
| (1,680) | 1:A:109:ALA:H | 1:A:109:ALA:HB2 | 20 | 0.14 |
| (1,670) | 1:A:106:ARG:H | 1:A:107:ASN:H | 12 | 0.14 |
| (1,663) | 1:A:104:PHE:H | 1:A:105:GLY:H | 3 | 0.14 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 14 | 0.14 |
| (1,651) | 1:A:99:ALA:H | 1:A:99:ALA:HB2 | 14 | 0.14 |
| (1,65) | 1:A:14:GLN:HA | 1:A:16:ASN:H | 19 | 0.14 |
| (1,648) | 1:A:98:LYS:HA | 1:A:99:ALA:H | 3 | 0.14 |
| (1,648) | 1:A:98:LYS:HA | 1:A:99:ALA:H | 19 | 0.14 |
| (1,64) | 1:A:14:GLN:HA | 1:A:15:GLY:H | 13 | 0.14 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 7 | 0.14 |
| (1,634) | 1:A:94:GLU:H | 1:A:95:GLN:H | 16 | 0.14 |
| (1,620) | 1:A:91:SER:H | 1:A:92:GLN:H | 12 | 0.14 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,62) | 1:A:14:GLN:HA | 1:A:14:GLN:HB2 | 14 | 0.14 |
| (1,604) | 1:A:85:GLU:H | 1:A:86:GLY:H | 5 | 0.14 |
| (1,604) | 1:A:85:GLU:H | 1:A:86:GLY:H | 11 | 0.14 |
| (1,599) | 1:A:83:ARG:HE | 1:A:84:TRP:H | 15 | 0.14 |
| (1,573) | 1:A:79:GLU:H | 1:A:80:GLN:H | 15 | 0.14 |
| (1,536) | 1:A:74:VAL:HG21 | 1:A:84:TRP:HZ3 | 15 | 0.14 |
| (1,53) | 1:A:13:TYR:H | 1:A:13:TYR:HA | 2 | 0.14 |
| (1,521) | 1:A:73:THR:HG1 | 1:A:74:VAL:H | 6 | 0.14 |
| (1,52) | 1:A:12:ILE:HG23 | 1:A:13:TYR:H | 14 | 0.14 |
| (1,517) | 1:A:73:THR:HA | 1:A:73:THR:HG1 | 19 | 0.14 |
| (1,514) | 1:A:73:THR:H | 1:A:73:THR:HB | 18 | 0.14 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 17 | 0.14 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 1 | 0.14 |
| (1,483) | 1:A:68:GLU:H | 1:A:69:ILE:H | 3 | 0.14 |
| (1,483) | 1:A:68:GLU:H | 1:A:69:ILE:H | 20 | 0.14 |
| (1,473) | 1:A:65:ALA:HB2 | 1:A:66:ARG:H | 14 | 0.14 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD12 | 13 | 0.14 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD22 | 13 | 0.14 |
| (1,446) | 1:A:61:VAL:H | 1:A:61:VAL:HB | 4 | 0.14 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 6 | 0.14 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 7 | 0.14 |
| (1,442) | 1:A:60:ARG:HA | 1:A:62:ASP:H | 10 | 0.14 |
| (1,433) | 1:A:59:GLN:H | 1:A:60:ARG:H | 13 | 0.14 |
| (1,432) | 1:A:58:THR:HG22 | 1:A:59:GLN:H | 19 | 0.14 |
| (1,424) | 1:A:58:THR:H | 1:A:59:GLN:H | 8 | 0.14 |
| (1,401) | 1:A:55:TYR:H | 1:A:55:TYR:HE1 | 20 | 0.14 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 15 | 0.14 |
| (1,384) | 1:A:53:TRP:H | 1:A:73:THR:HA | 1 | 0.14 |
| (1,360) | 1:A:52:ARG:H | 1:A:52:ARG:HA | 9 | 0.14 |
| (1,336) | 1:A:47:PRO:HA | 1:A:50:ALA:H | 1 | 0.14 |
| (1,323) | 1:A:44:ILE:HA | 1:A:44:ILE:HD12 | 4 | 0.14 |
| (1,32) | 1:A:9:LYS:H | 1:A:10:GLN:HA | 5 | 0.14 |
| (1,312) | 1:A:43:SER:H | 1:A:43:SER:HA | 12 | 0.14 |
| (1,312) | 1:A:43:SER:H | 1:A:43:SER:HA | 15 | 0.14 |
| (1,298) | 1:A:40:GLY:H | 1:A:41:THR:H | 15 | 0.14 |
| (1,286) | 1:A:39:LEU:H | 1:A:39:LEU:HG | 1 | 0.14 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 4 | 0.14 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 13 | 0.14 |
| (1,28) | 1:A:8:TYR:H | 1:A:8:TYR:HA | 12 | 0.14 |
| (1,28) | 1:A:8:TYR:H | 1:A:8:TYR:HA | 19 | 0.14 |
| (1,228) | 1:A:34:GLN:H | 1:A:36:SER:H | 8 | 0.14 |
| (1,228) | 1:A:34:GLN:H | 1:A:36:SER:H | 18 | 0.14 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,227) | 1:A:34:GLN:H | 1:A:35:VAL:H | 4 | 0.14 |
| (1,220) | 1:A:33:GLN:HA | 1:A:36:SER:H | 20 | 0.14 |
| (1,208) | 1:A:32:LYS:H | 1:A:33:GLN:H | 7 | 0.14 |
| (1,204) | 1:A:31:SER:HA | 1:A:80:GLN:HA | 20 | 0.14 |
| (1,199) | 1:A:31:SER:H | 1:A:81:VAL:H | 10 | 0.14 |
| (1,194) | 1:A:30:GLN:H | 1:A:81:VAL:H | 16 | 0.14 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 8 | 0.14 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 11 | 0.14 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 13 | 0.14 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 14 | 0.14 |
| (1,188) | 1:A:29:GLY:H | 1:A:30:GLN:H | 13 | 0.14 |
| (1,179) | 1:A:27:GLN:HB2 | 1:A:28:VAL:H | 4 | 0.14 |
| (1,152) | 1:A:26:LEU:H | 1:A:26:LEU:HA | 11 | 0.14 |
| (1,147) | 1:A:25:GLN:H | 1:A:26:LEU:H | 2 | 0.14 |
| (1,147) | 1:A:25:GLN:H | 1:A:26:LEU:H | 14 | 0.14 |
| (1,137) | 1:A:23:VAL:HG12 | 1:A:24:GLU:HA | 10 | 0.14 |
| (1,136) | 1:A:23:VAL:HG12 | 1:A:24:GLU:H | 6 | 0.14 |
| (1,135) | 1:A:23:VAL:HG11 | 1:A:84:TRP:HD1 | 13 | 0.14 |
| (1,135) | 1:A:23:VAL:HG11 | 1:A:84:TRP:HD1 | 20 | 0.14 |
| (1,111) | 1:A:21:ASN:HA | 1:A:24:GLU:H | 13 | 0.14 |
| (1,104) | 1:A:20:GLN:H | 1:A:21:ASN:H | 7 | 0.14 |
| (1,711) | 1:A:117:GLY:H | 1:A:118:ARG:H | 4 | 0.13 |
| (1,711) | 1:A:117:GLY:H | 1:A:118:ARG:H | 18 | 0.13 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 5 | 0.13 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 7 | 0.13 |
| (1,702) | 1:A:115:GLN:H | 1:A:115:GLN:HA | 20 | 0.13 |
| (1,699) | 1:A:113:LYS:HA | 1:A:114:LYS:H | 19 | 0.13 |
| (1,694) | 1:A:112:LYS:H | 1:A:112:LYS:HA | 4 | 0.13 |
| (1,694) | 1:A:112:LYS:H | 1:A:112:LYS:HA | 13 | 0.13 |
| (1,694) | 1:A:112:LYS:H | 1:A:112:LYS:HA | 19 | 0.13 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 11 | 0.13 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 13 | 0.13 |
| (1,681) | 1:A:109:ALA:H | 1:A:110:ARG:H | 5 | 0.13 |
| (1,676) | 1:A:108:LEU:H | 1:A:108:LEU:HA | 7 | 0.13 |
| (1,676) | 1:A:108:LEU:H | 1:A:108:LEU:HA | 18 | 0.13 |
| (1,655) | 1:A:100:ALA:H | 1:A:100:ALA:HB2 | 8 | 0.13 |
| (1,644) | 1:A:97:ALA:H | 1:A:97:ALA:HA | 19 | 0.13 |
| (1,644) | 1:A:97:ALA:H | 1:A:97:ALA:HA | 20 | 0.13 |
| (1,632) | 1:A:94:GLU:H | 1:A:94:GLU:HA | 11 | 0.13 |
| (1,626) | 1:A:92:GLN:HA | 1:A:93:ASP:H | 11 | 0.13 |
| (1,626) | 1:A:92:GLN:HA | 1:A:93:ASP:H | 17 | 0.13 |
| (1,618) | 1:A:90:PRO:HA | 1:A:91:SER:H | 1 | 0.13 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,597) | 1:A:83:ARG:HA | 1:A:84:TRP:H | 16 | 0.13 |
| (1,587) | 1:A:81:VAL:HG11 | 1:A:82:VAL:HA | 15 | 0.13 |
| (1,58) | 1:A:14:GLN:H | 1:A:14:GLN:HA | 4 | 0.13 |
| (1,554) | 1:A:76:PHE:HA | 1:A:81:VAL:HA | 13 | 0.13 |
| (1,552) | 1:A:76:PHE:HA | 1:A:78:ASN:H | 16 | 0.13 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 8 | 0.13 |
| (1,521) | 1:A:73:THR:HG1 | 1:A:74:VAL:H | 11 | 0.13 |
| (1,521) | 1:A:73:THR:HG1 | 1:A:74:VAL:H | 12 | 0.13 |
| (1,521) | 1:A:73:THR:HG1 | 1:A:74:VAL:H | 15 | 0.13 |
| (1,521) | 1:A:73:THR:HG1 | 1:A:74:VAL:H | 20 | 0.13 |
| (1,52) | 1:A:12:ILE:HG23 | 1:A:13:TYR:H | 8 | 0.13 |
| (1,52) | 1:A:12:ILE:HG23 | 1:A:13:TYR:H | 9 | 0.13 |
| (1,507) | 1:A:71:ASN:H | 1:A:88:TYR:HA | 2 | 0.13 |
| (1,506) | 1:A:71:ASN:H | 1:A:72:PHE:H | 17 | 0.13 |
| (1,506) | 1:A:71:ASN:H | 1:A:72:PHE:H | 20 | 0.13 |
| (1,491) | 1:A:69:ILE:HA | 1:A:69:ILE:HG22 | 19 | 0.13 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 6 | 0.13 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 7 | 0.13 |
| (1,474) | 1:A:66:ARG:H | 1:A:67:THR:H | 17 | 0.13 |
| (1,471) | 1:A:65:ALA:HA | 1:A:65:ALA:HB2 | 12 | 0.13 |
| (1,469) | 1:A:64:LEU:HD13 | 1:A:65:ALA:H | 7 | 0.13 |
| (1,465) | 1:A:64:LEU:H | 1:A:65:ALA:H | 16 | 0.13 |
| (1,462) | 1:A:64:LEU:H | 1:A:64:LEU:HA | 9 | 0.13 |
| (1,462) | 1:A:64:LEU:H | 1:A:64:LEU:HA | 12 | 0.13 |
| (1,456) | 1:A:62:ASP:HA | 1:A:63:ARG:H | 11 | 0.13 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 1 | 0.13 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 10 | 0.13 |
| (1,439) | 1:A:60:ARG:H | 1:A:61:VAL:H | 6 | 0.13 |
| (1,431) | 1:A:58:THR:HG1 | 1:A:59:GLN:H | 5 | 0.13 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG22 | 4 | 0.13 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG23 | 4 | 0.13 |
| (1,430) | 1:A:58:THR:HB | 1:A:69:ILE:HG21 | 4 | 0.13 |
| (1,43) | 1:A:12:ILE:H | 1:A:12:ILE:HA | 5 | 0.13 |
| (1,43) | 1:A:12:ILE:H | 1:A:12:ILE:HA | 11 | 0.13 |
| (1,43) | 1:A:12:ILE:H | 1:A:12:ILE:HA | 19 | 0.13 |
| (1,424) | 1:A:58:THR:H | 1:A:59:GLN:H | 2 | 0.13 |
| (1,418) | 1:A:57:SER:H | 1:A:71:ASN:HA | 14 | 0.13 |
| (1,408) | 1:A:56:THR:HA | 1:A:56:THR:HG21 | 16 | 0.13 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 13 | 0.13 |
| (1,370) | 1:A:52:ARG:HA | 1:A:76:PHE:HA | 2 | 0.13 |
| (1,360) | 1:A:52:ARG:H | 1:A:52:ARG:HA | 19 | 0.13 |
| (1,357) | 1:A:51:GLN:HA | 1:A:52:ARG:H | 7 | 0.13 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,345) | 1:A:49:HIS:HA | 1:A:49:HIS:HD2 | 14 | 0.13 |
| (1,345) | 1:A:49:HIS:HA | 1:A:49:HIS:HD2 | 19 | 0.13 |
| (1,336) | 1:A:47:PRO:HA | 1:A:50:ALA:H | 13 | 0.13 |
| (1,317) | 1:A:43:SER:HB2 | 1:A:44:ILE:H | 3 | 0.13 |
| (1,317) | 1:A:43:SER:HB3 | 1:A:44:ILE:H | 3 | 0.13 |
| (1,312) | 1:A:43:SER:H | 1:A:43:SER:HA | 1 | 0.13 |
| (1,312) | 1:A:43:SER:H | 1:A:43:SER:HA | 19 | 0.13 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 7 | 0.13 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 10 | 0.13 |
| (1,28) | 1:A:8:TYR:H | 1:A:8:TYR:HA | 7 | 0.13 |
| (1,28) | 1:A:8:TYR:H | 1:A:8:TYR:HA | 13 | 0.13 |
| (1,273) | 1:A:37:ALA:HA | 1:A:41:THR:H | 19 | 0.13 |
| (1,264) | 1:A:36:SER:HA | 1:A:53:TRP:HZ2 | 1 | 0.13 |
| (1,264) | 1:A:36:SER:HA | 1:A:53:TRP:HZ2 | 4 | 0.13 |
| (1,264) | 1:A:36:SER:HA | 1:A:53:TRP:HZ2 | 6 | 0.13 |
| (1,264) | 1:A:36:SER:HA | 1:A:53:TRP:HZ2 | 15 | 0.13 |
| (1,261) | 1:A:36:SER:HA | 1:A:39:LEU:H | 6 | 0.13 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 14 | 0.13 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 14 | 0.13 |
| (1,228) | 1:A:34:GLN:H | 1:A:36:SER:H | 13 | 0.13 |
| (1,227) | 1:A:34:GLN:H | 1:A:35:VAL:H | 14 | 0.13 |
| (1,221) | 1:A:33:GLN:HA | 1:A:37:ALA:H | 5 | 0.13 |
| (1,208) | 1:A:32:LYS:H | 1:A:33:GLN:H | 15 | 0.13 |
| (1,20) | 1:A:6:ILE:HA | 1:A:8:TYR:H | 17 | 0.13 |
| (1,199) | 1:A:31:SER:H | 1:A:81:VAL:H | 11 | 0.13 |
| (1,199) | 1:A:31:SER:H | 1:A:81:VAL:H | 16 | 0.13 |
| (1,169) | 1:A:26:LEU:HD12 | 1:A:84:TRP:HE3 | 3 | 0.13 |
| (1,152) | 1:A:26:LEU:H | 1:A:26:LEU:HA | 3 | 0.13 |
| (1,152) | 1:A:26:LEU:H | 1:A:26:LEU:HA | 14 | 0.13 |
| (1,152) | 1:A:26:LEU:H | 1:A:26:LEU:HA | 15 | 0.13 |
| (1,137) | 1:A:23:VAL:HG12 | 1:A:24:GLU:HA | 6 | 0.13 |
| (1,120) | 1:A:22:ALA:HA | 1:A:26:LEU:H | 3 | 0.13 |
| (1,111) | 1:A:21:ASN:HA | 1:A:24:GLU:H | 6 | 0.13 |
| (1,109) | 1:A:21:ASN:H | 1:A:23:VAL:H | 5 | 0.13 |
| (1,91) | 1:A:18:ILE:HD12 | 1:A:23:VAL:HG11 | 1 | 0.12 |
| (1,91) | 1:A:18:ILE:HD12 | 1:A:23:VAL:HG22 | 1 | 0.12 |
| (1,91) | 1:A:18:ILE:HD12 | 1:A:23:VAL:HG11 | 5 | 0.12 |
| (1,91) | 1:A:18:ILE:HD12 | 1:A:23:VAL:HG22 | 5 | 0.12 |
| (1,85) | 1:A:18:ILE:HA | 1:A:18:ILE:HG22 | 11 | 0.12 |
| (1,8) | 1:A:4:SER:H | 1:A:5:GLY:H | 6 | 0.12 |
| (1,707) | 1:A:116:ARG:H | 1:A:117:GLY:H | 17 | 0.12 |
| (1,704) | 1:A:115:GLN:H | 1:A:116:ARG:H | 1 | 0.12 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,697) | 1:A:112:LYS:HA | 1:A:113:LYS:H | 8 | 0.12 |
| (1,694) | 1:A:112:LYS:H | 1:A:112:LYS:HA | 20 | 0.12 |
| (1,681) | 1:A:109:ALA:H | 1:A:110:ARG:H | 2 | 0.12 |
| (1,676) | 1:A:108:LEU:H | 1:A:108:LEU:HA | 14 | 0.12 |
| (1,675) | 1:A:107:ASN:HA | 1:A:108:LEU:H | 13 | 0.12 |
| (1,674) | 1:A:107:ASN:H | 1:A:108:LEU:H | 4 | 0.12 |
| (1,671) | 1:A:106:ARG:HA | 1:A:107:ASN:H | 15 | 0.12 |
| (1,667) | 1:A:105:GLY:H | 1:A:106:ARG:H | 9 | 0.12 |
| (1,663) | 1:A:104:PHE:H | 1:A:105:GLY:H | 12 | 0.12 |
| (1,66) | 1:A:14:GLN:HB2 | 1:A:15:GLY:H | 4 | 0.12 |
| (1,64) | 1:A:14:GLN:HA | 1:A:15:GLY:H | 8 | 0.12 |
| (1,64) | 1:A:14:GLN:HA | 1:A:15:GLY:H | 15 | 0.12 |
| (1,638) | 1:A:95:GLN:H | 1:A:96:LEU:H | 11 | 0.12 |
| (1,634) | 1:A:94:GLU:H | 1:A:95:GLN:H | 9 | 0.12 |
| (1,620) | 1:A:91:SER:H | 1:A:92:GLN:H | 2 | 0.12 |
| (1,597) | 1:A:83:ARG:HA | 1:A:84:TRP:H | 18 | 0.12 |
| (1,597) | 1:A:83:ARG:HA | 1:A:84:TRP:H | 19 | 0.12 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG13 | 5 | 0.12 |
| (1,589) | 1:A:82:VAL:HA | 1:A:82:VAL:HG22 | 5 | 0.12 |
| (1,573) | 1:A:79:GLU:H | 1:A:80:GLN:H | 10 | 0.12 |
| (1,573) | 1:A:79:GLU:H | 1:A:80:GLN:H | 19 | 0.12 |
| (1,566) | 1:A:77:GLU:H | 1:A:81:VAL:HA | 5 | 0.12 |
| (1,566) | 1:A:77:GLU:H | 1:A:81:VAL:HA | 9 | 0.12 |
| (1,555) | 1:A:76:PHE:HA | 1:A:82:VAL:H | 19 | 0.12 |
| (1,554) | 1:A:76:PHE:HA | 1:A:81:VAL:HA | 5 | 0.12 |
| (1,536) | 1:A:74:VAL:HG21 | 1:A:84:TRP:HZ3 | 16 | 0.12 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 3 | 0.12 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 7 | 0.12 |
| (1,53) | 1:A:13:TYR:H | 1:A:13:TYR:HA | 15 | 0.12 |
| (1,53) | 1:A:13:TYR:H | 1:A:13:TYR:HA | 19 | 0.12 |
| (1,52) | 1:A:12:ILE:HG23 | 1:A:13:TYR:H | 11 | 0.12 |
| (1,504) | 1:A:70:LYS:HA | 1:A:89:PHE:H | 18 | 0.12 |
| (1,499) | 1:A:70:LYS:H | 1:A:71:ASN:H | 1 | 0.12 |
| (1,494) | 1:A:69:ILE:HB | 1:A:69:ILE:HD12 | 19 | 0.12 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 8 | 0.12 |
| (1,488) | 1:A:69:ILE:H | 1:A:69:ILE:HG23 | 16 | 0.12 |
| (1,470) | 1:A:65:ALA:H | 1:A:65:ALA:HB2 | 12 | 0.12 |
| (1,470) | 1:A:65:ALA:H | 1:A:65:ALA:HB3 | 12 | 0.12 |
| (1,469) | 1:A:64:LEU:HD13 | 1:A:65:ALA:H | 17 | 0.12 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD12 | 17 | 0.12 |
| (1,464) | 1:A:64:LEU:H | 1:A:64:LEU:HD22 | 17 | 0.12 |
| (1,452) | 1:A:61:VAL:HA | 1:A:62:ASP:H | 19 | 0.12 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 11 | 0.12 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 14 | 0.12 |
| (1,43) | 1:A:12:ILE:H | 1:A:12:ILE:HA | 4 | 0.12 |
| (1,424) | 1:A:58:THR:H | 1:A:59:GLN:H | 10 | 0.12 |
| (1,424) | 1:A:58:THR:H | 1:A:59:GLN:H | 11 | 0.12 |
| (1,424) | 1:A:58:THR:H | 1:A:59:GLN:H | 15 | 0.12 |
| (1,421) | 1:A:57:SER:HA | 1:A:58:THR:HB | 3 | 0.12 |
| (1,406) | 1:A:56:THR:H | 1:A:57:SER:H | 5 | 0.12 |
| (1,403) | 1:A:55:TYR:H | 1:A:73:THR:HA | 16 | 0.12 |
| (1,391) | 1:A:53:TRP:HE3 | 1:A:74:VAL:HG22 | 12 | 0.12 |
| (1,384) | 1:A:53:TRP:H | 1:A:73:THR:HA | 13 | 0.12 |
| (1,384) | 1:A:53:TRP:H | 1:A:73:THR:HA | 16 | 0.12 |
| (1,384) | 1:A:53:TRP:H | 1:A:73:THR:HA | 17 | 0.12 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 1 | 0.12 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 11 | 0.12 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 14 | 0.12 |
| (1,357) | 1:A:51:GLN:HA | 1:A:52:ARG:H | 13 | 0.12 |
| (1,35) | 1:A:9:LYS:HA | 1:A:10:GLN:H | 20 | 0.12 |
| (1,346) | 1:A:49:HIS:HA | 1:A:50:ALA:H | 4 | 0.12 |
| (1,336) | 1:A:47:PRO:HA | 1:A:50:ALA:H | 17 | 0.12 |
| (1,32) | 1:A:9:LYS:H | 1:A:10:GLN:HA | 4 | 0.12 |
| (1,32) | 1:A:9:LYS:H | 1:A:10:GLN:HA | 7 | 0.12 |
| (1,312) | 1:A:43:SER:H | 1:A:43:SER:HA | 3 | 0.12 |
| (1,312) | 1:A:43:SER:H | 1:A:43:SER:HA | 7 | 0.12 |
| (1,312) | 1:A:43:SER:H | 1:A:43:SER:HA | 9 | 0.12 |
| (1,298) | 1:A:40:GLY:H | 1:A:41:THR:H | 16 | 0.12 |
| (1,293) | 1:A:39:LEU:HD12 | 1:A:53:TRP:HH2 | 6 | 0.12 |
| (1,293) | 1:A:39:LEU:HD12 | 1:A:53:TRP:HH2 | 13 | 0.12 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 20 | 0.12 |
| (1,28) | 1:A:8:TYR:H | 1:A:8:TYR:HA | 9 | 0.12 |
| (1,28) | 1:A:8:TYR:H | 1:A:8:TYR:HA | 16 | 0.12 |
| (1,273) | 1:A:37:ALA:HA | 1:A:41:THR:H | 3 | 0.12 |
| (1,273) | 1:A:37:ALA:HA | 1:A:41:THR:H | 13 | 0.12 |
| (1,264) | 1:A:36:SER:HA | 1:A:53:TRP:HZ2 | 8 | 0.12 |
| (1,250) | 1:A:35:VAL:HG11 | 1:A:39:LEU:HD11 | 11 | 0.12 |
| (1,250) | 1:A:35:VAL:HG11 | 1:A:39:LEU:HD11 | 14 | 0.12 |
| (1,250) | 1:A:35:VAL:HG11 | 1:A:39:LEU:HD11 | 15 | 0.12 |
| (1,228) | 1:A:34:GLN:H | 1:A:36:SER:H | 1 | 0.12 |
| (1,228) | 1:A:34:GLN:H | 1:A:36:SER:H | 5 | 0.12 |
| (1,227) | 1:A:34:GLN:H | 1:A:35:VAL:H | 10 | 0.12 |
| (1,220) | 1:A:33:GLN:HA | 1:A:36:SER:H | 1 | 0.12 |
| (1,220) | 1:A:33:GLN:HA | 1:A:36:SER:H | 16 | 0.12 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,216) | 1:A:33:GLN:H | 1:A:35:VAL:H | 17 | 0.12 |
| (1,211) | 1:A:32:LYS:HA | 1:A:35:VAL:H | 13 | 0.12 |
| (1,209) | 1:A:32:LYS:H | 1:A:34:GLN:H | 7 | 0.12 |
| (1,209) | 1:A:32:LYS:H | 1:A:34:GLN:H | 17 | 0.12 |
| (1,207) | 1:A:32:LYS:H | 1:A:32:LYS:HA | 2 | 0.12 |
| (1,20) | 1:A:6:ILE:HA | 1:A:8:TYR:H | 8 | 0.12 |
| (1,20) | 1:A:6:ILE:HA | 1:A:8:TYR:H | 18 | 0.12 |
| (1,2) | 1:A:2:ALA:H | 1:A:3:GLY:H | 8 | 0.12 |
| (1,193) | 1:A:30:GLN:H | 1:A:31:SER:H | 13 | 0.12 |
| (1,189) | 1:A:29:GLY:H | 1:A:81:VAL:H | 10 | 0.12 |
| (1,184) | 1:A:28:VAL:HA | 1:A:30:GLN:H | 12 | 0.12 |
| (1,16) | 1:A:6:ILE:H | 1:A:7:ILE:H | 11 | 0.12 |
| (1,152) | 1:A:26:LEU:H | 1:A:26:LEU:HA | 6 | 0.12 |
| (1,151) | 1:A:25:GLN:HA | 1:A:27:GLN:H | 7 | 0.12 |
| (1,147) | 1:A:25:GLN:H | 1:A:26:LEU:H | 4 | 0.12 |
| (1,147) | 1:A:25:GLN:H | 1:A:26:LEU:H | 15 | 0.12 |
| (1,137) | 1:A:23:VAL:HG12 | 1:A:24:GLU:HA | 11 | 0.12 |
| (1,137) | 1:A:23:VAL:HG12 | 1:A:24:GLU:HA | 15 | 0.12 |
| (1,136) | 1:A:23:VAL:HG12 | 1:A:24:GLU:H | 13 | 0.12 |
| (1,120) | 1:A:22:ALA:HA | 1:A:26:LEU:H | 12 | 0.12 |
| (1,111) | 1:A:21:ASN:HA | 1:A:24:GLU:H | 4 | 0.12 |
| (1,101) | 1:A:20:GLN:H | 1:A:20:GLN:HA | 2 | 0.12 |
| (1,101) | 1:A:20:GLN:H | 1:A:20:GLN:HA | 15 | 0.12 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB3 | 14 | 0.12 |
| (1,1) | 1:A:1:MET:HA | 1:A:2:ALA:HB1 | 14 | 0.12 |
| (1,99) | 1:A:19:LYS:HA | 1:A:22:ALA:H | 16 | 0.11 |
| (1,85) | 1:A:18:ILE:HA | 1:A:18:ILE:HG22 | 2 | 0.11 |
| (1,78) | 1:A:17:LEU:HA | 1:A:18:ILE:H | 19 | 0.11 |
| (1,708) | 1:A:116:ARG:HA | 1:A:117:GLY:H | 14 | 0.11 |
| (1,700) | 1:A:114:LYS:H | 1:A:115:GLN:H | 2 | 0.11 |
| (1,70) | 1:A:16:ASN:H | 1:A:16:ASN:HA | 15 | 0.11 |
| (1,696) | 1:A:112:LYS:H | 1:A:113:LYS:H | 16 | 0.11 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 9 | 0.11 |
| (1,688) | 1:A:111:ASP:H | 1:A:111:ASP:HA | 12 | 0.11 |
| (1,687) | 1:A:110:ARG:HA | 1:A:111:ASP:H | 12 | 0.11 |
| (1,683) | 1:A:109:ALA:HB3 | 1:A:110:ARG:H | 5 | 0.11 |
| (1,683) | 1:A:109:ALA:HB1 | 1:A:110:ARG:H | 5 | 0.11 |
| (1,681) | 1:A:109:ALA:H | 1:A:110:ARG:H | 9 | 0.11 |
| (1,68) | 1:A:15:GLY:H | 1:A:16:ASN:H | 2 | 0.11 |
| (1,670) | 1:A:106:ARG:H | 1:A:107:ASN:H | 16 | 0.11 |
| (1,661) | 1:A:103:GLN:H | 1:A:104:PHE:H | 12 | 0.11 |
| (1,660) | 1:A:102:LYS:HA | 1:A:103:GLN:H | 1 | 0.11 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,651) | 1:A:99:ALA:H | 1:A:99:ALA:HB2 | 2 | 0.11 |
| (1,650) | 1:A:99:ALA:H | 1:A:99:ALA:HA | 2 | 0.11 |
| (1,650) | 1:A:99:ALA:H | 1:A:99:ALA:HA | 12 | 0.11 |
| (1,650) | 1:A:99:ALA:H | 1:A:99:ALA:HA | 14 | 0.11 |
| (1,645) | 1:A:97:ALA:H | 1:A:97:ALA:HB3 | 5 | 0.11 |
| (1,644) | 1:A:97:ALA:H | 1:A:97:ALA:HA | 15 | 0.11 |
| (1,626) | 1:A:92:GLN:HA | 1:A:93:ASP:H | 14 | 0.11 |
| (1,622) | 1:A:91:SER:HA | 1:A:92:GLN:H | 19 | 0.11 |
| (1,620) | 1:A:91:SER:H | 1:A:92:GLN:H | 20 | 0.11 |
| (1,618) | 1:A:90:PRO:HA | 1:A:91:SER:H | 18 | 0.11 |
| (1,61) | 1:A:14:GLN:H | 1:A:15:GLY:H | 13 | 0.11 |
| (1,604) | 1:A:85:GLU:H | 1:A:86:GLY:H | 3 | 0.11 |
| (1,604) | 1:A:85:GLU:H | 1:A:86:GLY:H | 18 | 0.11 |
| (1,588) | 1:A:82:VAL:H | 1:A:83:ARG:H | 18 | 0.11 |
| (1,588) | 1:A:82:VAL:H | 1:A:83:ARG:H | 19 | 0.11 |
| (1,587) | 1:A:81:VAL:HG11 | 1:A:82:VAL:HA | 8 | 0.11 |
| (1,587) | 1:A:81:VAL:HG11 | 1:A:82:VAL:HA | 18 | 0.11 |
| (1,573) | 1:A:79:GLU:H | 1:A:80:GLN:H | 2 | 0.11 |
| (1,573) | 1:A:79:GLU:H | 1:A:80:GLN:H | 6 | 0.11 |
| (1,573) | 1:A:79:GLU:H | 1:A:80:GLN:H | 17 | 0.11 |
| (1,573) | 1:A:79:GLU:H | 1:A:80:GLN:H | 20 | 0.11 |
| (1,57) | 1:A:13:TYR:HA | 1:A:14:GLN:H | 2 | 0.11 |
| (1,565) | 1:A:77:GLU:H | 1:A:80:GLN:H | 8 | 0.11 |
| (1,554) | 1:A:76:PHE:HA | 1:A:81:VAL:HA | 9 | 0.11 |
| (1,547) | 1:A:75:PHE:HD1 | 1:A:84:TRP:HA | 15 | 0.11 |
| (1,539) | 1:A:75:PHE:H | 1:A:84:TRP:HA | 19 | 0.11 |
| (1,533) | 1:A:74:VAL:HG11 | 1:A:84:TRP:HE3 | 1 | 0.11 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 6 | 0.11 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 12 | 0.11 |
| (1,531) | 1:A:74:VAL:HA | 1:A:85:GLU:H | 19 | 0.11 |
| (1,53) | 1:A:13:TYR:H | 1:A:13:TYR:HA | 10 | 0.11 |
| (1,521) | 1:A:73:THR:HG1 | 1:A:74:VAL:H | 13 | 0.11 |
| (1,512) | 1:A:72:PHE:HA | 1:A:87:ASP:H | 13 | 0.11 |
| (1,507) | 1:A:71:ASN:H | 1:A:88:TYR:HA | 16 | 0.11 |
| (1,494) | 1:A:69:ILE:HB | 1:A:69:ILE:HD12 | 8 | 0.11 |
| (1,477) | 1:A:67:THR:H | 1:A:67:THR:HB | 19 | 0.11 |
| (1,462) | 1:A:64:LEU:H | 1:A:64:LEU:HA | 11 | 0.11 |
| (1,462) | 1:A:64:LEU:H | 1:A:64:LEU:HA | 15 | 0.11 |
| (1,462) | 1:A:64:LEU:H | 1:A:64:LEU:HA | 19 | 0.11 |
| (1,446) | 1:A:61:VAL:H | 1:A:61:VAL:HB | 19 | 0.11 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 3 | 0.11 |
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 12 | 0.11 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,445) | 1:A:61:VAL:H | 1:A:61:VAL:HA | 20 | 0.11 |
| (1,432) | 1:A:58:THR:HG22 | 1:A:59:GLN:H | 3 | 0.11 |
| (1,431) | 1:A:58:THR:HG1 | 1:A:59:GLN:H | 4 | 0.11 |
| (1,43) | 1:A:12:ILE:H | 1:A:12:ILE:HA | 1 | 0.11 |
| (1,424) | 1:A:58:THR:H | 1:A:59:GLN:H | 17 | 0.11 |
| (1,424) | 1:A:58:THR:H | 1:A:59:GLN:H | 19 | 0.11 |
| (1,420) | 1:A:57:SER:HA | 1:A:58:THR:H | 11 | 0.11 |
| (1,42) | 1:A:11:PRO:HA | 1:A:12:ILE:H | 1 | 0.11 |
| (1,42) | 1:A:11:PRO:HA | 1:A:12:ILE:H | 14 | 0.11 |
| (1,42) | 1:A:11:PRO:HA | 1:A:12:ILE:H | 18 | 0.11 |
| (1,416) | 1:A:57:SER:H | 1:A:58:THR:H | 15 | 0.11 |
| (1,405) | 1:A:56:THR:H | 1:A:56:THR:HB | 6 | 0.11 |
| (1,405) | 1:A:56:THR:H | 1:A:56:THR:HB | 13 | 0.11 |
| (1,403) | 1:A:55:TYR:H | 1:A:73:THR:HA | 15 | 0.11 |
| (1,384) | 1:A:53:TRP:H | 1:A:73:THR:HA | 5 | 0.11 |
| (1,384) | 1:A:53:TRP:H | 1:A:73:THR:HA | 12 | 0.11 |
| (1,372) | 1:A:52:ARG:HB3 | 1:A:75:PHE:HA | 20 | 0.11 |
| (1,357) | 1:A:51:GLN:HA | 1:A:52:ARG:H | 1 | 0.11 |
| (1,345) | 1:A:49:HIS:HA | 1:A:49:HIS:HD2 | 16 | 0.11 |
| (1,339) | 1:A:48:PHE:H | 1:A:49:HIS:H | 6 | 0.11 |
| (1,331) | 1:A:45:PRO:HA | 1:A:46:ASP:H | 15 | 0.11 |
| (1,323) | 1:A:44:ILE:HA | 1:A:44:ILE:HD12 | 16 | 0.11 |
| (1,322) | 1:A:44:ILE:HA | 1:A:44:ILE:HG22 | 12 | 0.11 |
| (1,32) | 1:A:9:LYS:H | 1:A:10:GLN:HA | 20 | 0.11 |
| (1,314) | 1:A:43:SER:H | 1:A:44:ILE:H | 19 | 0.11 |
| (1,310) | 1:A:42:PRO:HA | 1:A:43:SER:H | 1 | 0.11 |
| (1,310) | 1:A:42:PRO:HA | 1:A:43:SER:H | 7 | 0.11 |
| (1,303) | 1:A:41:THR:HA | 1:A:41:THR:HG1 | 20 | 0.11 |
| (1,293) | 1:A:39:LEU:HD12 | 1:A:53:TRP:HH2 | 4 | 0.11 |
| (1,286) | 1:A:39:LEU:H | 1:A:39:LEU:HG | 19 | 0.11 |
| (1,282) | 1:A:38:LEU:HA | 1:A:40:GLY:H | 12 | 0.11 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD12 | 19 | 0.11 |
| (1,246) | 1:A:35:VAL:HA | 1:A:38:LEU:HD21 | 19 | 0.11 |
| (1,243) | 1:A:35:VAL:HA | 1:A:37:ALA:H | 5 | 0.11 |
| (1,243) | 1:A:35:VAL:HA | 1:A:37:ALA:H | 6 | 0.11 |
| (1,243) | 1:A:35:VAL:HA | 1:A:37:ALA:H | 8 | 0.11 |
| (1,228) | 1:A:34:GLN:H | 1:A:36:SER:H | 4 | 0.11 |
| (1,228) | 1:A:34:GLN:H | 1:A:36:SER:H | 10 | 0.11 |
| (1,215) | 1:A:33:GLN:H | 1:A:34:GLN:H | 1 | 0.11 |
| (1,211) | 1:A:32:LYS:HA | 1:A:35:VAL:H | 15 | 0.11 |
| (1,202) | 1:A:31:SER:HA | 1:A:33:GLN:H | 4 | 0.11 |
| (1,199) | 1:A:31:SER:H | 1:A:81:VAL:H | 8 | 0.11 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---|---|---|---|---|
| (1,199) | 1:A:31:SER:H | 1:A:81:VAL:H | 18 | 0.11 |
| (1,199) | 1:A:31:SER:H | 1:A:81:VAL:H | 19 | 0.11 |
| (1,193) | 1:A:30:GLN:H | 1:A:31:SER:H | 5 | 0.11 |
| (1,193) | 1:A:30:GLN:H | 1:A:31:SER:H | 9 | 0.11 |
| (1,193) | 1:A:30:GLN:H | 1:A:31:SER:H | 17 | 0.11 |
| (1,166) | 1:A:26:LEU:HG | 1:A:27:GLN:H | 20 | 0.11 |
| (1,161) | 1:A:26:LEU:HA | 1:A:28:VAL:H | 9 | 0.11 |
| (1,16) | 1:A:6:ILE:H | 1:A:7:ILE:H | 19 | 0.11 |
| (1,157) | 1:A:26:LEU:HA | 1:A:26:LEU:HB2 | 5 | 0.11 |
| (1,152) | 1:A:26:LEU:H | 1:A:26:LEU:HA | 13 | 0.11 |
| (1,147) | 1:A:25:GLN:H | 1:A:26:LEU:H | 10 | 0.11 |
| (1,147) | 1:A:25:GLN:H | 1:A:26:LEU:H | 17 | 0.11 |
| (1,147) | 1:A:25:GLN:H | 1:A:26:LEU:H | 20 | 0.11 |
| (1,126) | 1:A:23:VAL:H | 1:A:26:LEU:H | 13 | 0.11 |
| (1,122) | 1:A:23:VAL:H | 1:A:23:VAL:HB | 14 | 0.11 |
| (1,122) | 1:A:23:VAL:H | 1:A:23:VAL:HB | 19 | 0.11 |
| (1,111) | 1:A:21:ASN:HA | 1:A:24:GLU:H | 19 | 0.11 |
| (1,110) | 1:A:21:ASN:H | 1:A:24:GLU:H | 11 | 0.11 |
| (1,101) | 1:A:20:GLN:H | 1:A:20:GLN:HA | 7 | 0.11 |
| (1,101) | 1:A:20:GLN:H | 1:A:20:GLN:HA | 9 | 0.11 |

# 10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found