



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 11:16 PM UTC

PDB ID : 2MZV / pdb\_00002mzv  
BMRB ID : 19689  
Title : Resonance assignments and secondary structure of a phytocystatin from Sesamum indicum  
Authors : Chyan, C.  
Deposited on : 2015-02-25

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

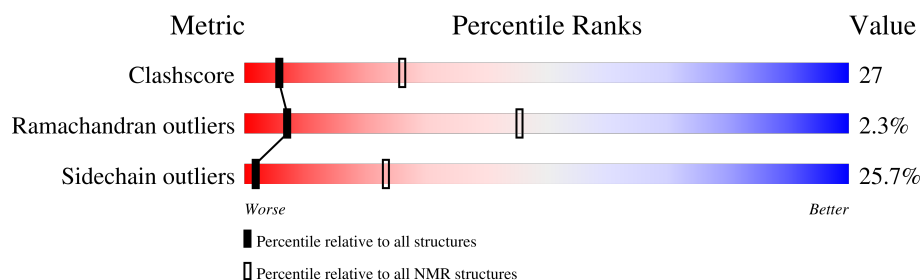
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 87%.

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



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

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

| Mol | Chain | Length | Quality of chain                                                                    |
|-----|-------|--------|-------------------------------------------------------------------------------------|
| 1   | A     | 199    | <div> <div></div> <div>36%</div> <div>39%</div> <div>8%</div> <div>18%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:3-A:91 (89)                                 | 0.58              | 1            |
| 2                                    | A:112-A:137, A:144-A:183,<br>A:189-A:197 (75) | 0.21              | 13           |

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3148 atoms, of which 1571 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cystatin.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 199      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 3148  | 994 | 1571 | 280 | 300 | 3 |       |

## 4 Residue-property plots [i](#)

### 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.

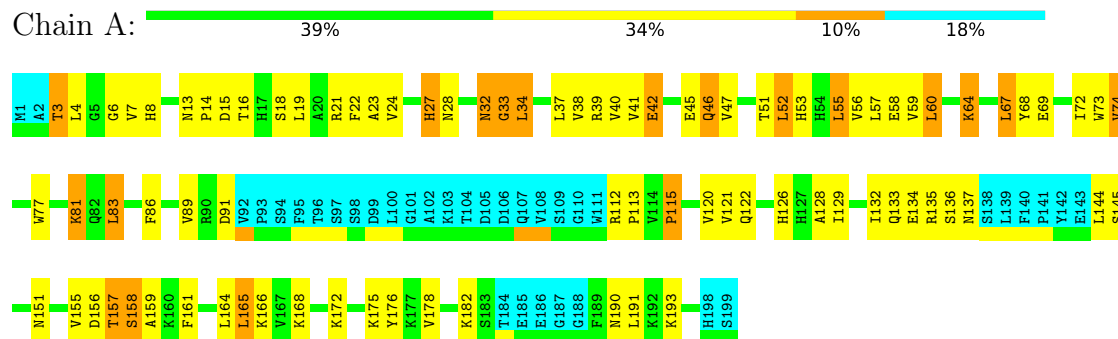
- Molecule 1: Cystatin



Colouring as in section 4.1 above.

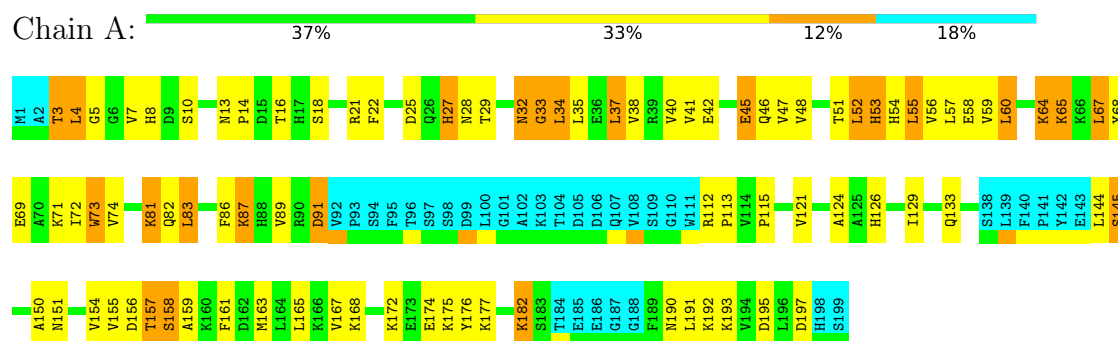
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Cystatin



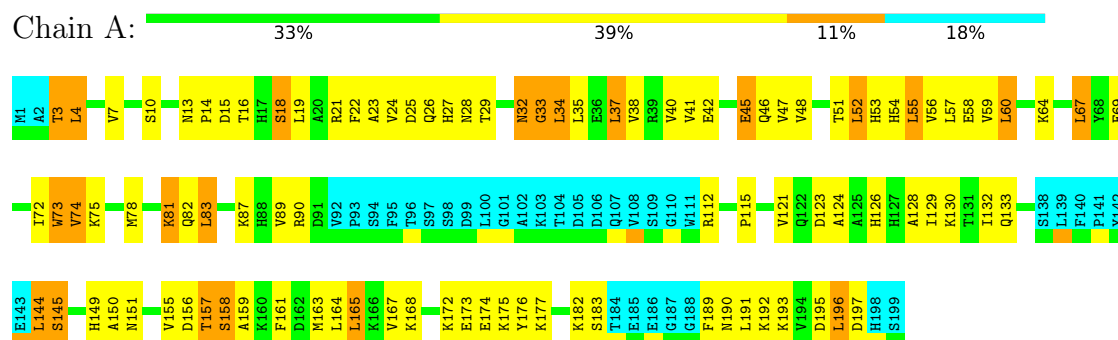
## 4.2.2 Score per residue for model 2

### • Molecule 1: Cystatin



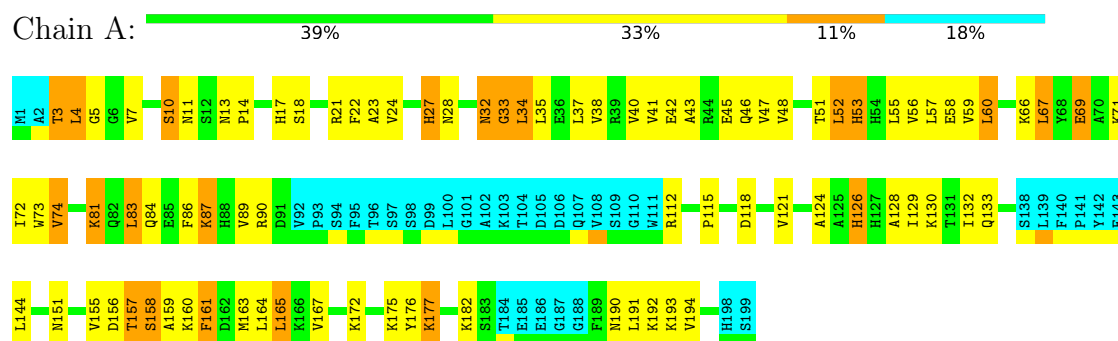
## 4.2.3 Score per residue for model 3

### • Molecule 1: Cystatin



## 4.2.4 Score per residue for model 4

### • Molecule 1: Cystatin

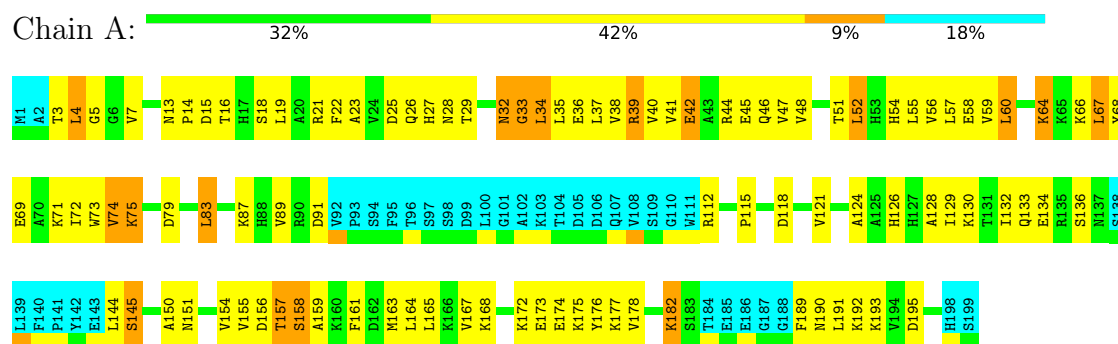






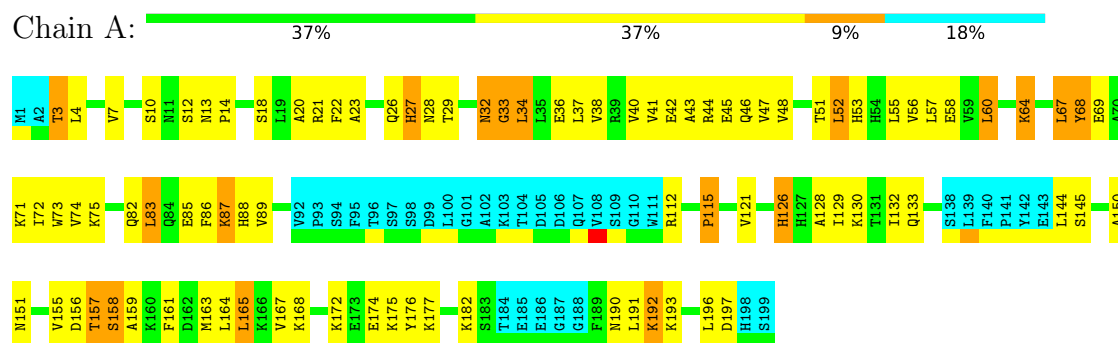
## 4.2.11 Score per residue for model 11

## • Molecule 1: Cystatin



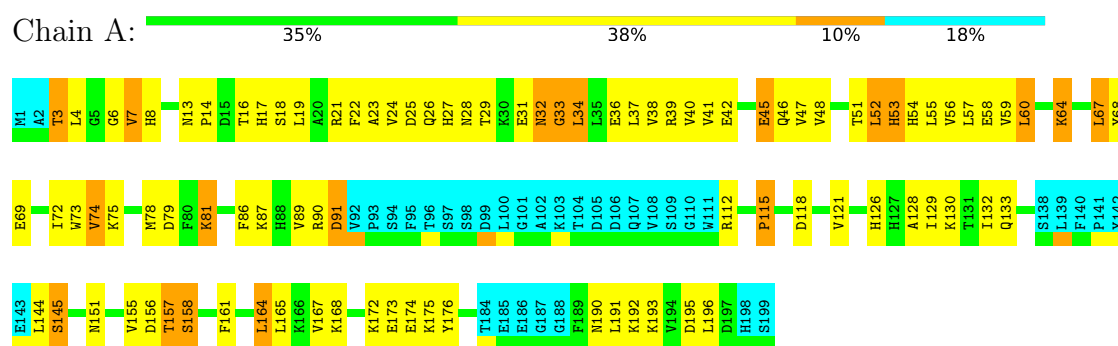
## 4.2.12 Score per residue for model 12

## • Molecule 1: Cystatin



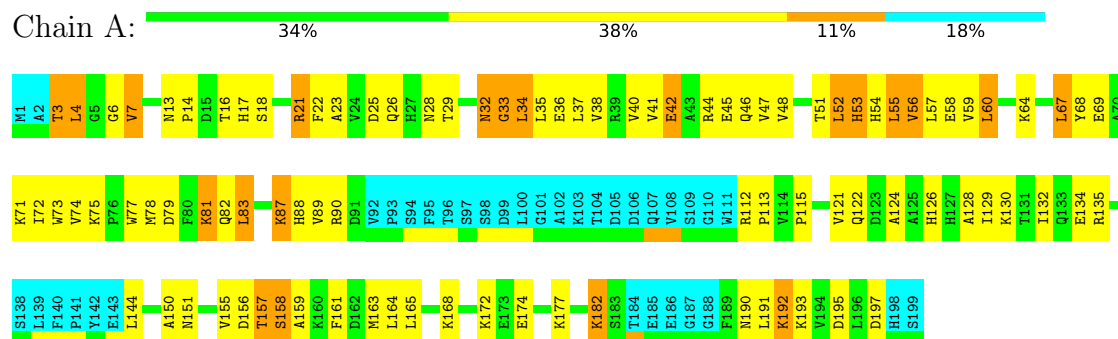
## 4.2.13 Score per residue for model 13

## • Molecule 1: Cystatin



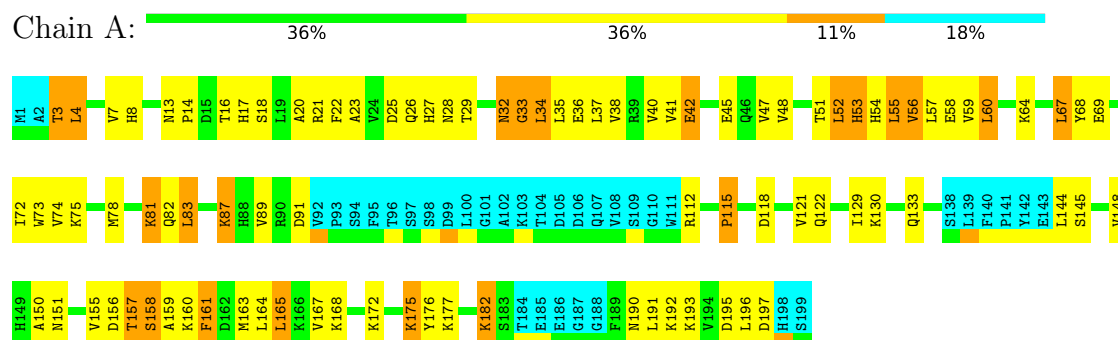
## 4.2.14 Score per residue for model 14

## • Molecule 1: Cystatin



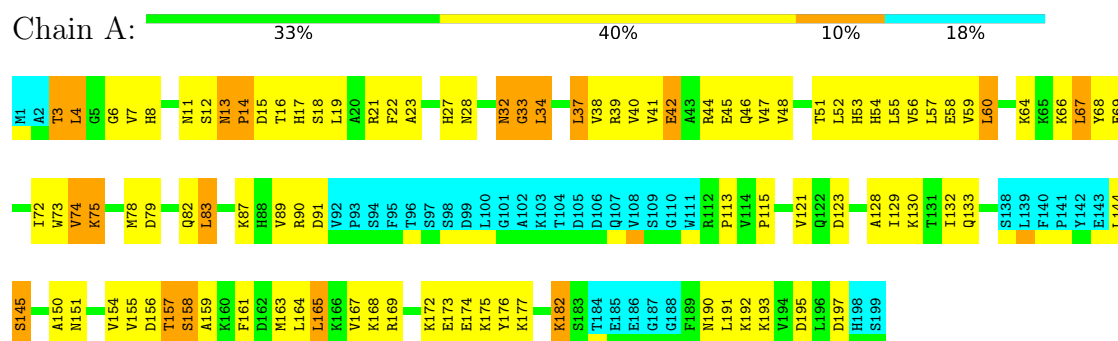
## 4.2.15 Score per residue for model 15

## • Molecule 1: Cystatin



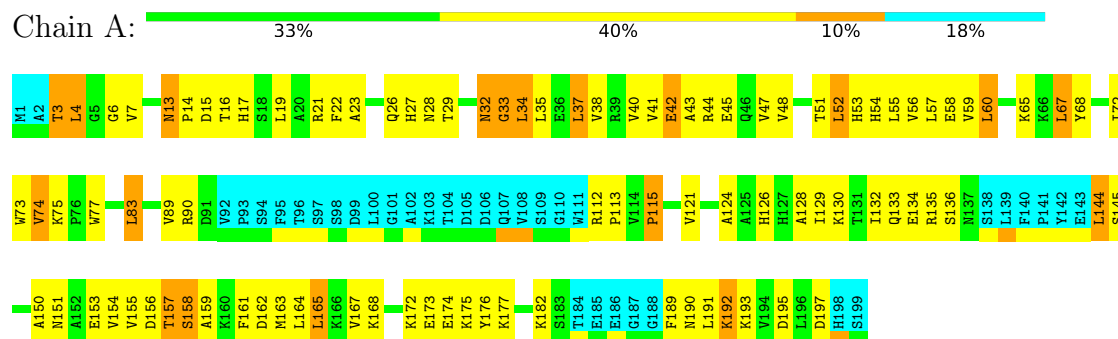
## 4.2.16 Score per residue for model 16

## • Molecule 1: Cystatin



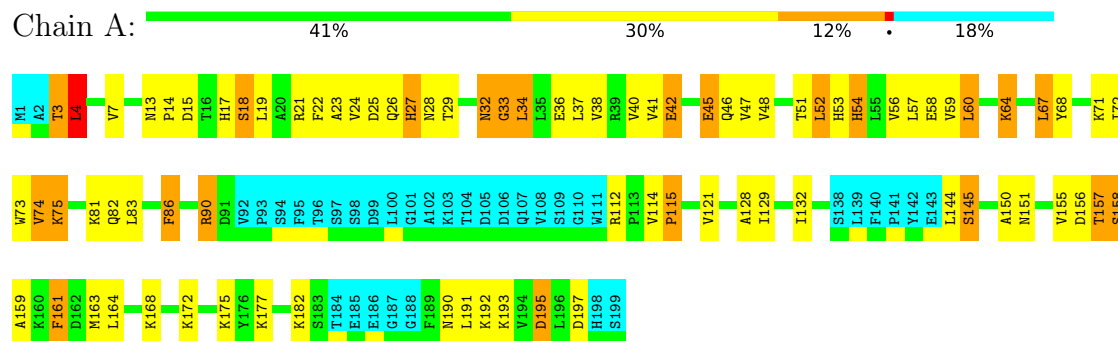
## 4.2.17 Score per residue for model 17

## • Molecule 1: Cystatin



## 4.2.18 Score per residue for model 18

## • Molecule 1: Cystatin



## 4.2.19 Score per residue for model 19

## • Molecule 1: Cystatin



## 4.2.20 Score per residue for model 20

### ● Molecule 1: Cystatin



## 5 Refinement protocol and experimental data overview

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

Of the 400 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 |
|---------------|--------------------|---------|
| CYANA         | structure solution | 2.1     |
| CNSSLVE       | refinement         | 1.2     |
| CYANA         | refinement         | 2.1     |

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                       | 2353           |
| Number of shifts mapped to atoms             | 2353           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 87%            |

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1315  | 1339     | 1328     | 72±6    |
| All | All   | 26300 | 26780    | 26560    | 1434    |

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 27.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:129:ILE:HD11 | 1:A:165:LEU:HD11 | 1.03     | 1.27        | 1      | 12    |
| 1:A:3:THR:HG22   | 1:A:51:THR:HG21  | 1.00     | 1.29        | 3      | 8     |
| 1:A:52:LEU:HD12  | 1:A:73:TRP:CH2   | 0.89     | 2.01        | 19     | 5     |
| 1:A:17:HIS:CD2   | 1:A:40:VAL:HG21  | 0.88     | 2.03        | 14     | 2     |
| 1:A:38:VAL:HG21  | 1:A:60:LEU:HD23  | 0.85     | 1.48        | 1      | 6     |
| 1:A:129:ILE:CD1  | 1:A:165:LEU:HD11 | 0.83     | 2.03        | 1      | 1     |
| 1:A:4:LEU:HD11   | 1:A:53:HIS:CE1   | 0.83     | 2.08        | 13     | 2     |
| 1:A:4:LEU:HD21   | 1:A:53:HIS:ND1   | 0.80     | 1.90        | 13     | 3     |
| 1:A:46:GLN:CB    | 1:A:52:LEU:HD12  | 0.78     | 2.09        | 20     | 2     |
| 1:A:56:VAL:HG22  | 1:A:69:GLU:CG    | 0.77     | 2.09        | 10     | 1     |
| 1:A:161:PHE:CD1  | 1:A:163:MET:HE3  | 0.77     | 2.13        | 15     | 2     |
| 1:A:17:HIS:CE1   | 1:A:40:VAL:HG21  | 0.77     | 2.14        | 17     | 3     |
| 1:A:52:LEU:HD23  | 1:A:73:TRP:CZ3   | 0.77     | 2.14        | 20     | 3     |
| 1:A:52:LEU:O     | 1:A:52:LEU:HD13  | 0.76     | 1.81        | 20     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:3:THR:C      | 1:A:4:LEU:HD13   | 0.76     | 2.06        | 3      | 10    |
| 1:A:58:GLU:HG3   | 1:A:67:LEU:HD22  | 0.75     | 1.57        | 4      | 2     |
| 1:A:69:GLU:CD    | 1:A:89:VAL:HG11  | 0.74     | 2.07        | 16     | 7     |
| 1:A:51:THR:HB    | 1:A:74:VAL:HG13  | 0.74     | 1.59        | 9      | 11    |
| 1:A:52:LEU:HD12  | 1:A:53:HIS:N     | 0.74     | 1.97        | 2      | 10    |
| 1:A:52:LEU:HD13  | 1:A:73:TRP:CZ3   | 0.73     | 2.18        | 12     | 8     |
| 1:A:52:LEU:HD22  | 1:A:53:HIS:N     | 0.73     | 1.98        | 4      | 3     |
| 1:A:46:GLN:HB3   | 1:A:52:LEU:HD12  | 0.73     | 1.60        | 1      | 3     |
| 1:A:58:GLU:HG2   | 1:A:67:LEU:HD22  | 0.73     | 1.61        | 17     | 18    |
| 1:A:4:LEU:HD12   | 1:A:45:GLU:CD    | 0.72     | 2.09        | 13     | 3     |
| 1:A:41:VAL:HG23  | 1:A:57:LEU:HA    | 0.72     | 1.61        | 4      | 20    |
| 1:A:155:VAL:HG12 | 1:A:158:SER:O    | 0.72     | 1.85        | 6      | 19    |
| 1:A:164:LEU:HD12 | 1:A:176:TYR:O    | 0.71     | 1.86        | 15     | 11    |
| 1:A:3:THR:HG22   | 1:A:51:THR:OG1   | 0.71     | 1.86        | 9      | 8     |
| 1:A:41:VAL:HG22  | 1:A:58:GLU:OE2   | 0.71     | 1.86        | 1      | 2     |
| 1:A:69:GLU:OE1   | 1:A:89:VAL:HG11  | 0.70     | 1.86        | 4      | 7     |
| 1:A:38:VAL:CG2   | 1:A:60:LEU:HD23  | 0.70     | 2.17        | 4      | 6     |
| 1:A:23:ALA:HB2   | 1:A:83:LEU:HD22  | 0.70     | 1.63        | 1      | 6     |
| 1:A:46:GLN:HB3   | 1:A:52:LEU:HD22  | 0.70     | 1.63        | 18     | 2     |
| 1:A:7:VAL:HG23   | 1:A:45:GLU:O     | 0.69     | 1.88        | 8      | 3     |
| 1:A:58:GLU:CG    | 1:A:67:LEU:HD22  | 0.69     | 2.17        | 4      | 7     |
| 1:A:155:VAL:HG12 | 1:A:158:SER:C    | 0.69     | 2.13        | 11     | 19    |
| 1:A:56:VAL:HG22  | 1:A:69:GLU:HG2   | 0.68     | 1.64        | 13     | 3     |
| 1:A:167:VAL:HG22 | 1:A:174:GLU:O    | 0.68     | 1.88        | 9      | 8     |
| 1:A:129:ILE:HD13 | 1:A:176:TYR:OH   | 0.68     | 1.88        | 9      | 12    |
| 1:A:52:LEU:C     | 1:A:52:LEU:HD23  | 0.67     | 2.14        | 17     | 5     |
| 1:A:72:ILE:CD1   | 1:A:83:LEU:HD23  | 0.67     | 2.19        | 11     | 17    |
| 1:A:41:VAL:HG23  | 1:A:57:LEU:CA    | 0.66     | 2.21        | 17     | 20    |
| 1:A:144:LEU:HD23 | 1:A:145:SER:N    | 0.66     | 2.05        | 11     | 9     |
| 1:A:122:GLN:NE2  | 1:A:144:LEU:HD21 | 0.65     | 2.06        | 1      | 4     |
| 1:A:37:LEU:HA    | 1:A:59:VAL:HG12  | 0.65     | 1.68        | 3      | 16    |
| 1:A:52:LEU:HD22  | 1:A:72:ILE:O     | 0.65     | 1.91        | 9      | 1     |
| 1:A:21:ARG:HD3   | 1:A:37:LEU:HD22  | 0.65     | 1.65        | 19     | 20    |
| 1:A:126:HIS:CD2  | 1:A:144:LEU:HD23 | 0.65     | 2.27        | 6      | 4     |
| 1:A:51:THR:CG2   | 1:A:74:VAL:HG13  | 0.65     | 2.22        | 19     | 11    |
| 1:A:16:THR:HB    | 1:A:55:LEU:HD21  | 0.65     | 1.67        | 1      | 5     |
| 1:A:72:ILE:HG12  | 1:A:83:LEU:HD23  | 0.65     | 1.67        | 1      | 12    |
| 1:A:74:VAL:HG13  | 1:A:81:LYS:HA    | 0.65     | 1.69        | 5      | 8     |
| 1:A:67:LEU:HD23  | 1:A:67:LEU:N     | 0.64     | 2.07        | 17     | 20    |
| 1:A:167:VAL:HG13 | 1:A:176:TYR:CE1  | 0.64     | 2.27        | 7      | 3     |
| 1:A:52:LEU:HD12  | 1:A:73:TRP:CZ3   | 0.64     | 2.27        | 19     | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:10:SER:OG    | 1:A:43:ALA:HB3   | 0.64     | 1.93        | 8      | 2     |
| 1:A:17:HIS:CG    | 1:A:40:VAL:HG21  | 0.64     | 2.27        | 14     | 1     |
| 1:A:4:LEU:HD13   | 1:A:4:LEU:N      | 0.63     | 2.09        | 14     | 13    |
| 1:A:52:LEU:HD23  | 1:A:73:TRP:CD1   | 0.63     | 2.28        | 9      | 2     |
| 1:A:49:ALA:HB3   | 1:A:73:TRP:CH2   | 0.62     | 2.30        | 7      | 1     |
| 1:A:60:LEU:HD23  | 1:A:64:LYS:N     | 0.62     | 2.09        | 14     | 14    |
| 1:A:42:GLU:HG2   | 1:A:56:VAL:HG13  | 0.62     | 1.69        | 20     | 6     |
| 1:A:41:VAL:HG12  | 1:A:42:GLU:CD    | 0.62     | 2.19        | 16     | 7     |
| 1:A:52:LEU:HD22  | 1:A:52:LEU:C     | 0.62     | 2.19        | 20     | 3     |
| 1:A:16:THR:HB    | 1:A:55:LEU:HD13  | 0.62     | 1.70        | 16     | 4     |
| 1:A:150:ALA:HB1  | 1:A:163:MET:HE2  | 0.62     | 1.72        | 15     | 2     |
| 1:A:69:GLU:OE2   | 1:A:89:VAL:HG11  | 0.62     | 1.94        | 13     | 4     |
| 1:A:164:LEU:HD13 | 1:A:177:LYS:HD2  | 0.61     | 1.71        | 9      | 14    |
| 1:A:48:VAL:HG11  | 1:A:73:TRP:CZ2   | 0.61     | 2.29        | 13     | 11    |
| 1:A:25:ASP:O     | 1:A:29:THR:HG22  | 0.60     | 1.97        | 19     | 13    |
| 1:A:56:VAL:HG22  | 1:A:69:GLU:HG3   | 0.60     | 1.74        | 10     | 1     |
| 1:A:15:ASP:O     | 1:A:19:LEU:HD23  | 0.60     | 1.97        | 17     | 9     |
| 1:A:33:GLY:C     | 1:A:34:LEU:HD13  | 0.60     | 2.22        | 7      | 20    |
| 1:A:115:PRO:O    | 1:A:121:VAL:HG21 | 0.59     | 1.96        | 4      | 14    |
| 1:A:23:ALA:HA    | 1:A:83:LEU:HD22  | 0.59     | 1.74        | 20     | 3     |
| 1:A:24:VAL:HG21  | 1:A:37:LEU:HD11  | 0.59     | 1.71        | 18     | 7     |
| 1:A:121:VAL:HG13 | 1:A:163:MET:SD   | 0.59     | 2.37        | 2      | 11    |
| 1:A:42:GLU:HG2   | 1:A:56:VAL:CG1   | 0.59     | 2.27        | 17     | 6     |
| 1:A:4:LEU:HD23   | 1:A:51:THR:HG21  | 0.59     | 1.73        | 20     | 2     |
| 1:A:34:LEU:N     | 1:A:34:LEU:HD13  | 0.58     | 2.14        | 2      | 8     |
| 1:A:3:THR:HG22   | 1:A:51:THR:CB    | 0.58     | 2.29        | 10     | 2     |
| 1:A:40:VAL:HG22  | 1:A:57:LEU:HD12  | 0.58     | 1.74        | 9      | 12    |
| 1:A:72:ILE:HG21  | 1:A:81:LYS:HD2   | 0.58     | 1.75        | 13     | 1     |
| 1:A:165:LEU:HD11 | 1:A:176:TYR:OH   | 0.58     | 1.98        | 19     | 2     |
| 1:A:124:ALA:HB3  | 1:A:163:MET:HE1  | 0.57     | 1.77        | 14     | 3     |
| 1:A:21:ARG:CD    | 1:A:37:LEU:HD22  | 0.57     | 2.30        | 5      | 11    |
| 1:A:34:LEU:HD13  | 1:A:34:LEU:N     | 0.57     | 2.14        | 19     | 12    |
| 1:A:165:LEU:HD23 | 1:A:165:LEU:N    | 0.57     | 2.15        | 20     | 1     |
| 1:A:72:ILE:CG1   | 1:A:83:LEU:HD23  | 0.57     | 2.29        | 1      | 12    |
| 1:A:52:LEU:HD13  | 1:A:52:LEU:C     | 0.57     | 2.25        | 4      | 3     |
| 1:A:3:THR:C      | 1:A:4:LEU:HD22   | 0.57     | 2.24        | 13     | 1     |
| 1:A:74:VAL:HG13  | 1:A:81:LYS:CA    | 0.56     | 2.30        | 14     | 8     |
| 1:A:4:LEU:HD22   | 1:A:51:THR:HG23  | 0.56     | 1.76        | 10     | 1     |
| 1:A:159:ALA:HB3  | 1:A:182:LYS:HB2  | 0.56     | 1.78        | 12     | 18    |
| 1:A:7:VAL:HG22   | 1:A:46:GLN:HA    | 0.56     | 1.77        | 4      | 7     |
| 1:A:176:TYR:HB3  | 1:A:196:LEU:HD13 | 0.56     | 1.78        | 19     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:7:VAL:O      | 1:A:7:VAL:HG13   | 0.56     | 2.00        | 14     | 3     |
| 1:A:48:VAL:HG11  | 1:A:73:TRP:CH2   | 0.56     | 2.35        | 3      | 4     |
| 1:A:46:GLN:CB    | 1:A:52:LEU:HD22  | 0.56     | 2.31        | 11     | 1     |
| 1:A:4:LEU:HD22   | 1:A:4:LEU:N      | 0.56     | 2.16        | 4      | 3     |
| 1:A:51:THR:CB    | 1:A:74:VAL:HG13  | 0.56     | 2.31        | 9      | 11    |
| 1:A:38:VAL:HG22  | 1:A:60:LEU:HD12  | 0.55     | 1.77        | 13     | 14    |
| 1:A:155:VAL:HG22 | 1:A:160:LYS:HG3  | 0.55     | 1.77        | 8      | 1     |
| 1:A:46:GLN:HB3   | 1:A:52:LEU:HD23  | 0.55     | 1.77        | 14     | 3     |
| 1:A:7:VAL:HG13   | 1:A:45:GLU:O     | 0.55     | 2.01        | 3      | 2     |
| 1:A:16:THR:HG21  | 1:A:43:ALA:HB2   | 0.55     | 1.78        | 20     | 1     |
| 1:A:4:LEU:HD12   | 1:A:45:GLU:OE2   | 0.55     | 2.02        | 1      | 2     |
| 1:A:37:LEU:HD23  | 1:A:57:LEU:HD13  | 0.55     | 1.78        | 20     | 11    |
| 1:A:155:VAL:HG13 | 1:A:157:THR:H    | 0.55     | 1.61        | 12     | 19    |
| 1:A:52:LEU:HD13  | 1:A:73:TRP:HZ3   | 0.55     | 1.58        | 13     | 10    |
| 1:A:3:THR:CG2    | 1:A:51:THR:HG21  | 0.55     | 2.31        | 5      | 2     |
| 1:A:48:VAL:O     | 1:A:48:VAL:HG13  | 0.54     | 2.02        | 10     | 9     |
| 1:A:26:GLN:O     | 1:A:29:THR:HG22  | 0.54     | 2.03        | 17     | 4     |
| 1:A:41:VAL:HG22  | 1:A:58:GLU:CG    | 0.54     | 2.33        | 2      | 12    |
| 1:A:72:ILE:HG23  | 1:A:82:GLN:C     | 0.54     | 2.28        | 9      | 12    |
| 1:A:59:VAL:HG13  | 1:A:68:TYR:CE1   | 0.54     | 2.38        | 19     | 17    |
| 1:A:23:ALA:CA    | 1:A:83:LEU:HD22  | 0.54     | 2.33        | 20     | 9     |
| 1:A:20:ALA:HB1   | 1:A:68:TYR:OH    | 0.54     | 2.03        | 9      | 3     |
| 1:A:124:ALA:HB2  | 1:A:189:PHE:CZ   | 0.53     | 2.38        | 3      | 4     |
| 1:A:3:THR:HG23   | 1:A:74:VAL:CG1   | 0.53     | 2.32        | 5      | 4     |
| 1:A:72:ILE:HD11  | 1:A:83:LEU:HD23  | 0.53     | 1.80        | 20     | 16    |
| 1:A:41:VAL:HG23  | 1:A:57:LEU:C     | 0.53     | 2.29        | 17     | 19    |
| 1:A:52:LEU:C     | 1:A:52:LEU:HD13  | 0.53     | 2.29        | 9      | 2     |
| 1:A:163:MET:O    | 1:A:178:VAL:HG22 | 0.53     | 2.04        | 11     | 3     |
| 1:A:3:THR:HG22   | 1:A:51:THR:HB    | 0.52     | 1.80        | 20     | 2     |
| 1:A:7:VAL:HG12   | 1:A:7:VAL:O      | 0.52     | 2.03        | 16     | 5     |
| 1:A:47:VAL:O     | 1:A:47:VAL:HG13  | 0.52     | 2.05        | 2      | 20    |
| 1:A:3:THR:HG23   | 1:A:74:VAL:HG11  | 0.52     | 1.80        | 14     | 6     |
| 1:A:48:VAL:HG12  | 1:A:73:TRP:CZ2   | 0.52     | 2.38        | 7      | 1     |
| 1:A:161:PHE:CE1  | 1:A:163:MET:HE3  | 0.52     | 2.40        | 15     | 2     |
| 1:A:41:VAL:HG22  | 1:A:58:GLU:HG3   | 0.51     | 1.81        | 10     | 9     |
| 1:A:24:VAL:CG2   | 1:A:37:LEU:HD11  | 0.51     | 2.35        | 18     | 5     |
| 1:A:52:LEU:HD23  | 1:A:73:TRP:HZ3   | 0.51     | 1.64        | 20     | 3     |
| 1:A:4:LEU:HD22   | 1:A:4:LEU:H      | 0.51     | 1.64        | 5      | 4     |
| 1:A:28:ASN:HA    | 1:A:32:ASN:HB3   | 0.51     | 1.83        | 20     | 20    |
| 1:A:164:LEU:HD23 | 1:A:176:TYR:O    | 0.51     | 2.06        | 13     | 1     |
| 1:A:144:LEU:HD13 | 1:A:165:LEU:HD22 | 0.51     | 1.82        | 14     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:38:VAL:HG12  | 1:A:39:ARG:HD3   | 0.50     | 1.81        | 11     | 1     |
| 1:A:155:VAL:HG22 | 1:A:156:ASP:H    | 0.50     | 1.66        | 4      | 19    |
| 1:A:4:LEU:HD13   | 1:A:45:GLU:OE2   | 0.50     | 2.06        | 18     | 1     |
| 1:A:36:GLU:CG    | 1:A:60:LEU:HB2   | 0.50     | 2.36        | 7      | 14    |
| 1:A:86:PHE:N     | 1:A:86:PHE:CD1   | 0.50     | 2.80        | 18     | 2     |
| 1:A:32:ASN:ND2   | 1:A:35:LEU:HD12  | 0.50     | 2.22        | 15     | 6     |
| 1:A:176:TYR:CB   | 1:A:196:LEU:HD13 | 0.50     | 2.37        | 6      | 7     |
| 1:A:52:LEU:HD23  | 1:A:52:LEU:O     | 0.50     | 2.06        | 17     | 5     |
| 1:A:4:LEU:CD2    | 1:A:51:THR:HG23  | 0.50     | 2.36        | 10     | 1     |
| 1:A:53:HIS:CE1   | 1:A:72:ILE:HD12  | 0.50     | 2.42        | 18     | 3     |
| 1:A:129:ILE:HD11 | 1:A:165:LEU:CD1  | 0.50     | 2.18        | 1      | 3     |
| 1:A:167:VAL:HG13 | 1:A:176:TYR:HE1  | 0.50     | 1.66        | 19     | 3     |
| 1:A:42:GLU:H     | 1:A:56:VAL:HG13  | 0.50     | 1.66        | 12     | 5     |
| 1:A:191:LEU:C    | 1:A:191:LEU:HD13 | 0.50     | 2.32        | 16     | 20    |
| 1:A:38:VAL:CG2   | 1:A:60:LEU:HD12  | 0.50     | 2.37        | 7      | 13    |
| 1:A:129:ILE:HD13 | 1:A:144:LEU:N    | 0.50     | 2.22        | 8      | 3     |
| 1:A:12:SER:OG    | 1:A:40:VAL:HG21  | 0.50     | 2.07        | 12     | 1     |
| 1:A:155:VAL:HG23 | 1:A:160:LYS:HE2  | 0.50     | 1.83        | 15     | 2     |
| 1:A:52:LEU:HD12  | 1:A:52:LEU:C     | 0.49     | 2.32        | 13     | 9     |
| 1:A:144:LEU:HD12 | 1:A:165:LEU:HD13 | 0.49     | 1.83        | 19     | 1     |
| 1:A:161:PHE:CD1  | 1:A:163:MET:HE2  | 0.49     | 2.42        | 4      | 1     |
| 1:A:23:ALA:HA    | 1:A:83:LEU:HD13  | 0.49     | 1.83        | 1      | 1     |
| 1:A:12:SER:HA    | 1:A:16:THR:HG23  | 0.49     | 1.85        | 20     | 1     |
| 1:A:20:ALA:HB3   | 1:A:37:LEU:HD21  | 0.49     | 1.85        | 12     | 1     |
| 1:A:72:ILE:HG21  | 1:A:81:LYS:HD3   | 0.48     | 1.84        | 4      | 1     |
| 1:A:23:ALA:CB    | 1:A:83:LEU:HD22  | 0.48     | 2.34        | 1      | 2     |
| 1:A:87:LYS:HE2   | 1:A:89:VAL:HG13  | 0.48     | 1.86        | 14     | 3     |
| 1:A:4:LEU:HD11   | 1:A:53:HIS:HB2   | 0.48     | 1.84        | 18     | 1     |
| 1:A:41:VAL:HB    | 1:A:56:VAL:HG13  | 0.48     | 1.84        | 17     | 5     |
| 1:A:52:LEU:HD13  | 1:A:53:HIS:N     | 0.48     | 2.23        | 9      | 1     |
| 1:A:125:ALA:HB1  | 1:A:165:LEU:CD2  | 0.48     | 2.38        | 10     | 1     |
| 1:A:87:LYS:NZ    | 1:A:89:VAL:HG12  | 0.48     | 2.24        | 8      | 1     |
| 1:A:22:PHE:O     | 1:A:83:LEU:HD13  | 0.48     | 2.08        | 3      | 2     |
| 1:A:42:GLU:N     | 1:A:56:VAL:HG13  | 0.48     | 2.23        | 12     | 4     |
| 1:A:59:VAL:CG1   | 1:A:68:TYR:CE1   | 0.47     | 2.97        | 9      | 13    |
| 1:A:86:PHE:CD1   | 1:A:86:PHE:N     | 0.47     | 2.82        | 20     | 2     |
| 1:A:17:HIS:ND1   | 1:A:40:VAL:HG21  | 0.47     | 2.22        | 17     | 1     |
| 1:A:52:LEU:C     | 1:A:52:LEU:CD2   | 0.47     | 2.88        | 11     | 5     |
| 1:A:4:LEU:O      | 1:A:51:THR:HG23  | 0.47     | 2.09        | 1      | 2     |
| 1:A:53:HIS:ND1   | 1:A:72:ILE:HD12  | 0.47     | 2.25        | 18     | 2     |
| 1:A:60:LEU:HD13  | 1:A:64:LYS:N     | 0.47     | 2.25        | 3      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:51:THR:CG2   | 1:A:74:VAL:CG1   | 0.47     | 2.92        | 20     | 11    |
| 1:A:41:VAL:HG22  | 1:A:58:GLU:HG2   | 0.46     | 1.87        | 16     | 4     |
| 1:A:191:LEU:HD13 | 1:A:192:LYS:N    | 0.46     | 2.25        | 16     | 19    |
| 1:A:14:PRO:HG2   | 1:A:16:THR:HG23  | 0.46     | 1.87        | 17     | 2     |
| 1:A:114:VAL:HG21 | 1:A:163:MET:HE2  | 0.46     | 1.86        | 18     | 1     |
| 1:A:148:VAL:HG21 | 1:A:175:LYS:HD2  | 0.46     | 1.88        | 15     | 1     |
| 1:A:40:VAL:HA    | 1:A:57:LEU:HD12  | 0.46     | 1.86        | 12     | 8     |
| 1:A:72:ILE:HG23  | 1:A:83:LEU:HA    | 0.46     | 1.86        | 9      | 8     |
| 1:A:150:ALA:HB1  | 1:A:163:MET:SD   | 0.46     | 2.50        | 14     | 15    |
| 1:A:51:THR:HG22  | 1:A:74:VAL:HG13  | 0.46     | 1.88        | 19     | 2     |
| 1:A:10:SER:HB2   | 1:A:43:ALA:HB3   | 0.46     | 1.88        | 4      | 1     |
| 1:A:22:PHE:CD1   | 1:A:22:PHE:N     | 0.46     | 2.82        | 12     | 19    |
| 1:A:4:LEU:HD12   | 1:A:45:GLU:CG    | 0.45     | 2.40        | 1      | 1     |
| 1:A:35:LEU:HD22  | 1:A:59:VAL:HG21  | 0.45     | 1.88        | 17     | 1     |
| 1:A:17:HIS:CD2   | 1:A:40:VAL:CG1   | 0.45     | 3.00        | 4      | 2     |
| 1:A:126:HIS:CE1  | 1:A:144:LEU:CB   | 0.45     | 3.00        | 2      | 5     |
| 1:A:176:TYR:CE2  | 1:A:178:VAL:CG1  | 0.45     | 3.00        | 9      | 2     |
| 1:A:41:VAL:HB    | 1:A:56:VAL:HG22  | 0.45     | 1.87        | 19     | 4     |
| 1:A:54:HIS:CE1   | 1:A:71:LYS:CE    | 0.45     | 3.00        | 18     | 1     |
| 1:A:17:HIS:CG    | 1:A:40:VAL:CG2   | 0.45     | 3.00        | 15     | 1     |
| 1:A:161:PHE:CE1  | 1:A:163:MET:CE   | 0.45     | 3.00        | 18     | 2     |
| 1:A:128:ALA:O    | 1:A:132:ILE:HD12 | 0.45     | 2.12        | 12     | 18    |
| 1:A:13:ASN:CB    | 1:A:14:PRO:HD3   | 0.45     | 2.42        | 10     | 2     |
| 1:A:60:LEU:HD21  | 1:A:65:LYS:CD    | 0.45     | 2.42        | 2      | 1     |
| 1:A:13:ASN:CB    | 1:A:14:PRO:CD    | 0.44     | 2.95        | 17     | 16    |
| 1:A:17:HIS:NE2   | 1:A:40:VAL:HG11  | 0.44     | 2.27        | 4      | 1     |
| 1:A:23:ALA:O     | 1:A:26:GLN:CG    | 0.44     | 2.66        | 18     | 8     |
| 1:A:40:VAL:CG2   | 1:A:57:LEU:HD12  | 0.44     | 2.42        | 3      | 1     |
| 1:A:177:LYS:O    | 1:A:194:VAL:HG23 | 0.44     | 2.12        | 4      | 1     |
| 1:A:4:LEU:N      | 1:A:4:LEU:HD22   | 0.44     | 2.28        | 5      | 1     |
| 1:A:49:ALA:CB    | 1:A:73:TRP:CH2   | 0.44     | 3.00        | 7      | 1     |
| 1:A:48:VAL:HG12  | 1:A:52:LEU:HB3   | 0.44     | 1.90        | 6      | 4     |
| 1:A:144:LEU:CD1  | 1:A:165:LEU:HD13 | 0.44     | 2.42        | 19     | 3     |
| 1:A:155:VAL:HG23 | 1:A:159:ALA:HA   | 0.44     | 1.89        | 8      | 1     |
| 1:A:52:LEU:CD2   | 1:A:73:TRP:CD1   | 0.44     | 2.99        | 9      | 1     |
| 1:A:24:VAL:HG21  | 1:A:37:LEU:CD1   | 0.44     | 2.42        | 18     | 1     |
| 1:A:52:LEU:CD1   | 1:A:73:TRP:CH2   | 0.43     | 2.95        | 16     | 1     |
| 1:A:176:TYR:HB2  | 1:A:196:LEU:HD13 | 0.43     | 1.89        | 20     | 4     |
| 1:A:51:THR:HG22  | 1:A:74:VAL:CG1   | 0.43     | 2.43        | 19     | 5     |
| 1:A:13:ASN:N     | 1:A:14:PRO:CD    | 0.43     | 2.81        | 8      | 4     |
| 1:A:144:LEU:HG   | 1:A:165:LEU:HD13 | 0.43     | 1.89        | 17     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:17:HIS:CD2   | 1:A:57:LEU:CD1   | 0.43     | 3.02        | 5      | 2     |
| 1:A:148:VAL:HG21 | 1:A:175:LYS:NZ   | 0.43     | 2.29        | 20     | 1     |
| 1:A:16:THR:CB    | 1:A:55:LEU:HD21  | 0.43     | 2.44        | 15     | 2     |
| 1:A:68:TYR:HA    | 1:A:89:VAL:HG22  | 0.43     | 1.90        | 5      | 2     |
| 1:A:67:LEU:N     | 1:A:67:LEU:CD2   | 0.42     | 2.82        | 9      | 5     |
| 1:A:4:LEU:N      | 1:A:4:LEU:CD1    | 0.42     | 2.81        | 17     | 7     |
| 1:A:20:ALA:CB    | 1:A:37:LEU:HD21  | 0.42     | 2.44        | 12     | 1     |
| 1:A:48:VAL:HG12  | 1:A:52:LEU:CB    | 0.42     | 2.44        | 6      | 4     |
| 1:A:72:ILE:HG23  | 1:A:83:LEU:CA    | 0.42     | 2.44        | 9      | 1     |
| 1:A:19:LEU:HB3   | 1:A:55:LEU:HD12  | 0.42     | 1.91        | 13     | 1     |
| 1:A:3:THR:HG22   | 1:A:51:THR:CG2   | 0.42     | 2.38        | 5      | 2     |
| 1:A:17:HIS:CD2   | 1:A:40:VAL:HG11  | 0.42     | 2.49        | 8      | 1     |
| 1:A:161:PHE:CG   | 1:A:163:MET:HE2  | 0.42     | 2.49        | 4      | 1     |
| 1:A:67:LEU:O     | 1:A:89:VAL:HG22  | 0.42     | 2.15        | 17     | 1     |
| 1:A:27:HIS:CB    | 1:A:86:PHE:CZ    | 0.42     | 3.03        | 2      | 2     |
| 1:A:74:VAL:CG2   | 1:A:75:LYS:N     | 0.42     | 2.83        | 11     | 7     |
| 1:A:12:SER:HB3   | 1:A:40:VAL:HG11  | 0.42     | 1.92        | 19     | 1     |
| 1:A:177:LYS:N    | 1:A:195:ASP:O    | 0.42     | 2.53        | 14     | 10    |
| 1:A:52:LEU:CD1   | 1:A:73:TRP:CZ3   | 0.41     | 3.02        | 11     | 2     |
| 1:A:4:LEU:HD23   | 1:A:51:THR:CG2   | 0.41     | 2.44        | 12     | 2     |
| 1:A:68:TYR:O     | 1:A:68:TYR:CD1   | 0.41     | 2.72        | 12     | 1     |
| 1:A:18:SER:CB    | 1:A:22:PHE:CZ    | 0.41     | 3.04        | 3      | 1     |
| 1:A:17:HIS:CE1   | 1:A:40:VAL:CG2   | 0.41     | 3.03        | 18     | 1     |
| 1:A:35:LEU:HD21  | 1:A:66:LYS:NZ    | 0.41     | 2.30        | 4      | 1     |
| 1:A:126:HIS:CD2  | 1:A:144:LEU:HD13 | 0.41     | 2.49        | 9      | 1     |
| 1:A:3:THR:HG21   | 1:A:76:PRO:CG    | 0.41     | 2.45        | 10     | 1     |
| 1:A:68:TYR:CD1   | 1:A:68:TYR:C     | 0.41     | 2.98        | 12     | 1     |
| 1:A:40:VAL:CA    | 1:A:57:LEU:HD12  | 0.41     | 2.45        | 4      | 2     |
| 1:A:27:HIS:HB2   | 1:A:86:PHE:CZ    | 0.41     | 2.50        | 1      | 6     |
| 1:A:34:LEU:N     | 1:A:34:LEU:CD1   | 0.41     | 2.84        | 2      | 2     |
| 1:A:120:VAL:HG13 | 1:A:121:VAL:N    | 0.41     | 2.31        | 10     | 1     |
| 1:A:132:ILE:HG23 | 1:A:194:VAL:HG11 | 0.41     | 1.92        | 19     | 1     |
| 1:A:18:SER:O     | 1:A:22:PHE:CE1   | 0.41     | 2.74        | 18     | 1     |
| 1:A:132:ILE:HD11 | 1:A:178:VAL:HG23 | 0.41     | 1.92        | 1      | 1     |
| 1:A:129:ILE:CD1  | 1:A:144:LEU:CA   | 0.41     | 2.99        | 8      | 2     |
| 1:A:144:LEU:HD23 | 1:A:145:SER:H    | 0.41     | 1.76        | 3      | 3     |
| 1:A:129:ILE:CD1  | 1:A:144:LEU:N    | 0.41     | 2.84        | 14     | 4     |
| 1:A:72:ILE:HG23  | 1:A:83:LEU:N     | 0.41     | 2.31        | 9      | 2     |
| 1:A:54:HIS:CD2   | 1:A:69:GLU:CD    | 0.41     | 2.99        | 19     | 1     |
| 1:A:7:VAL:O      | 1:A:8:HIS:CG     | 0.41     | 2.74        | 7      | 3     |
| 1:A:17:HIS:ND1   | 1:A:40:VAL:CG2   | 0.41     | 2.84        | 18     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:7:VAL:HG23  | 1:A:46:GLN:HG3  | 0.40     | 1.93        | 14     | 1     |
| 1:A:43:ALA:CB   | 1:A:55:LEU:CD2  | 0.40     | 2.99        | 17     | 1     |
| 1:A:54:HIS:CE1  | 1:A:71:LYS:HE2  | 0.40     | 2.51        | 18     | 1     |
| 1:A:20:ALA:O    | 1:A:24:VAL:HG23 | 0.40     | 2.16        | 5      | 1     |
| 1:A:48:VAL:HG12 | 1:A:52:LEU:HB2  | 0.40     | 1.93        | 19     | 1     |
| 1:A:32:ASN:ND2  | 1:A:35:LEU:CD1  | 0.40     | 2.85        | 2      | 1     |
| 1:A:88:HIS:O    | 1:A:88:HIS:CD2  | 0.40     | 2.75        | 7      | 2     |
| 1:A:149:HIS:CD2 | 1:A:149:HIS:O   | 0.40     | 2.75        | 3      | 1     |
| 1:A:87:LYS:NZ   | 1:A:89:VAL:CG1  | 0.40     | 2.84        | 15     | 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     | 164/199 (82%)   | 137±2 (84±1%) | 23±2 (14±1%) | 4±1 (2±1%) | 7           | 45 |
| All | All   | 3280/3980 (82%) | 2739 (84%)    | 464 (14%)    | 77 (2%)    | 7           | 45 |

All 14 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     | 33  | GLY  | 20             |
| 1   | A     | 115 | PRO  | 19             |
| 1   | A     | 113 | PRO  | 7              |
| 1   | A     | 6   | GLY  | 6              |
| 1   | A     | 8   | HIS  | 4              |
| 1   | A     | 90  | ARG  | 4              |
| 1   | A     | 7   | VAL  | 4              |
| 1   | A     | 5   | GLY  | 3              |
| 1   | A     | 91  | ASP  | 3              |
| 1   | A     | 4   | LEU  | 2              |
| 1   | A     | 13  | ASN  | 2              |
| 1   | A     | 10  | SER  | 1              |
| 1   | A     | 78  | MET  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 14  | PRO  | 1              |

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed        | Rotameric     | Outliers     | Percentiles |    |
|-----|-------|-----------------|---------------|--------------|-------------|----|
| 1   | A     | 145/174 (83%)   | 108±4 (74±3%) | 37±4 (26±3%) | 2           | 23 |
| All | All   | 2900/3480 (83%) | 2156 (74%)    | 744 (26%)    | 2           | 23 |

All 83 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     | 3   | THR  | 20             |
| 1   | A     | 32  | ASN  | 20             |
| 1   | A     | 34  | LEU  | 20             |
| 1   | A     | 60  | LEU  | 20             |
| 1   | A     | 67  | LEU  | 20             |
| 1   | A     | 151 | ASN  | 20             |
| 1   | A     | 158 | SER  | 20             |
| 1   | A     | 161 | PHE  | 20             |
| 1   | A     | 172 | LYS  | 20             |
| 1   | A     | 190 | ASN  | 20             |
| 1   | A     | 193 | LYS  | 20             |
| 1   | A     | 42  | GLU  | 18             |
| 1   | A     | 175 | LYS  | 18             |
| 1   | A     | 27  | HIS  | 17             |
| 1   | A     | 52  | LEU  | 17             |
| 1   | A     | 83  | LEU  | 17             |
| 1   | A     | 145 | SER  | 17             |
| 1   | A     | 157 | THR  | 17             |
| 1   | A     | 168 | LYS  | 17             |
| 1   | A     | 45  | GLU  | 17             |
| 1   | A     | 112 | ARG  | 16             |
| 1   | A     | 54  | HIS  | 16             |
| 1   | A     | 87  | LYS  | 16             |
| 1   | A     | 18  | SER  | 15             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 4   | LEU  | 15             |
| 1   | A     | 165 | LEU  | 13             |
| 1   | A     | 197 | ASP  | 13             |
| 1   | A     | 130 | LYS  | 13             |
| 1   | A     | 74  | VAL  | 11             |
| 1   | A     | 81  | LYS  | 11             |
| 1   | A     | 53  | HIS  | 11             |
| 1   | A     | 64  | LYS  | 10             |
| 1   | A     | 195 | ASP  | 10             |
| 1   | A     | 118 | ASP  | 10             |
| 1   | A     | 55  | LEU  | 9              |
| 1   | A     | 75  | LYS  | 9              |
| 1   | A     | 173 | GLU  | 9              |
| 1   | A     | 71  | LYS  | 8              |
| 1   | A     | 182 | LYS  | 8              |
| 1   | A     | 78  | MET  | 8              |
| 1   | A     | 90  | ARG  | 8              |
| 1   | A     | 44  | ARG  | 8              |
| 1   | A     | 39  | ARG  | 6              |
| 1   | A     | 126 | HIS  | 6              |
| 1   | A     | 8   | HIS  | 5              |
| 1   | A     | 136 | SER  | 5              |
| 1   | A     | 164 | LEU  | 5              |
| 1   | A     | 73  | TRP  | 5              |
| 1   | A     | 79  | ASP  | 5              |
| 1   | A     | 56  | VAL  | 5              |
| 1   | A     | 135 | ARG  | 4              |
| 1   | A     | 166 | LYS  | 4              |
| 1   | A     | 37  | LEU  | 4              |
| 1   | A     | 65  | LYS  | 4              |
| 1   | A     | 177 | LYS  | 4              |
| 1   | A     | 144 | LEU  | 4              |
| 1   | A     | 192 | LYS  | 4              |
| 1   | A     | 46  | GLN  | 3              |
| 1   | A     | 77  | TRP  | 3              |
| 1   | A     | 120 | VAL  | 3              |
| 1   | A     | 123 | ASP  | 3              |
| 1   | A     | 11  | ASN  | 3              |
| 1   | A     | 69  | GLU  | 3              |
| 1   | A     | 66  | LYS  | 3              |
| 1   | A     | 91  | ASP  | 3              |
| 1   | A     | 86  | PHE  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 10  | SER  | 2              |
| 1   | A     | 174 | GLU  | 2              |
| 1   | A     | 127 | HIS  | 2              |
| 1   | A     | 169 | ARG  | 2              |
| 1   | A     | 15  | ASP  | 2              |
| 1   | A     | 31  | GLU  | 2              |
| 1   | A     | 21  | ARG  | 2              |
| 1   | A     | 162 | ASP  | 2              |
| 1   | A     | 134 | GLU  | 1              |
| 1   | A     | 183 | SER  | 1              |
| 1   | A     | 196 | LEU  | 1              |
| 1   | A     | 84  | GLN  | 1              |
| 1   | A     | 68  | TYR  | 1              |
| 1   | A     | 12  | SER  | 1              |
| 1   | A     | 153 | GLU  | 1              |
| 1   | A     | 82  | GLN  | 1              |
| 1   | A     | 88  | HIS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 86% 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                  | 2353 |
| Number of shifts mapped to atoms        | 2353 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 2    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 194      | $-0.15 \pm 0.09$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 184      | $-0.01 \pm 0.06$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 194      | $0.10 \pm 0.06$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 190      | $-0.53 \pm 0.18$                | 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 87%, i.e. 2004 atoms were assigned a chemical shift out of a possible 2312. 0 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|---------------|-----------------|-----------------|
| Backbone  | 809/817 (99%)   | 327/330 (99%) | 324/328 (99%)   | 158/159 (99%)   |
| Sidechain | 1142/1315 (87%) | 781/851 (92%) | 351/412 (85%)   | 10/52 (19%)     |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 53/180 (29%)    | 51/89 (57%)          | 0/67 (0%)             | 2/24 (8%)             |
| Overall  | 2004/2312 (87%) | 1159/1270 (91%)      | 675/807 (84%)         | 170/235 (72%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 2353 atoms were assigned a chemical shift out of a possible 2725. 0 out of 43 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 974/992 (98%)   | 396/402 (99%)        | 388/398 (97%)         | 190/192 (99%)         |
| Sidechain | 1307/1504 (87%) | 893/974 (92%)        | 403/476 (85%)         | 11/54 (20%)           |
| Aromatic  | 72/229 (31%)    | 69/113 (61%)         | 0/89 (0%)             | 3/27 (11%)            |
| Overall   | 2353/2725 (86%) | 1358/1489 (91%)      | 791/963 (82%)         | 204/273 (75%)         |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

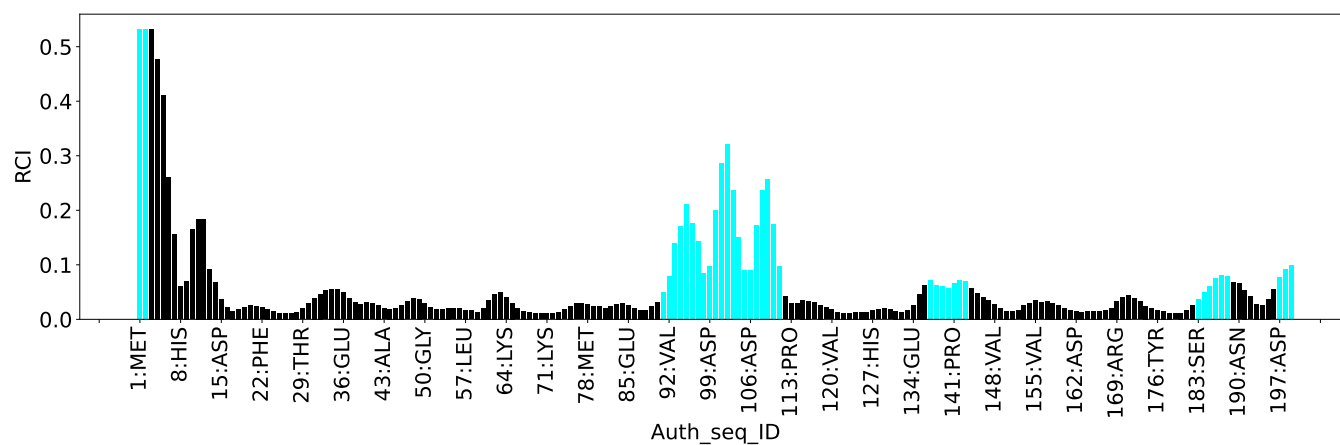
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 153 | GLU  | HB3  | 0.27       | 0.95 – 3.05         | -8.2    |
| 1       | A     | 153 | GLU  | HB2  | 0.71       | 1.00 – 3.05         | -6.4    |

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 2769  |
| Intra-residue ( $ i-j =0$ )                              | 552   |
| Sequential ( $ i-j =1$ )                                 | 838   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 403   |
| Long range ( $ i-j \geq 5$ )                             | 976   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 226   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 15.1  |
| Number of long range restraints per residue <sup>1</sup> | 4.9   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 4.0                                    | 0.2     |
| 0.2-0.5 (Medium) | 4.8                                    | 0.5     |
| >0.5 (Large)     | 76.2                                   | 6.88    |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 2.4                                    | 1.91    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

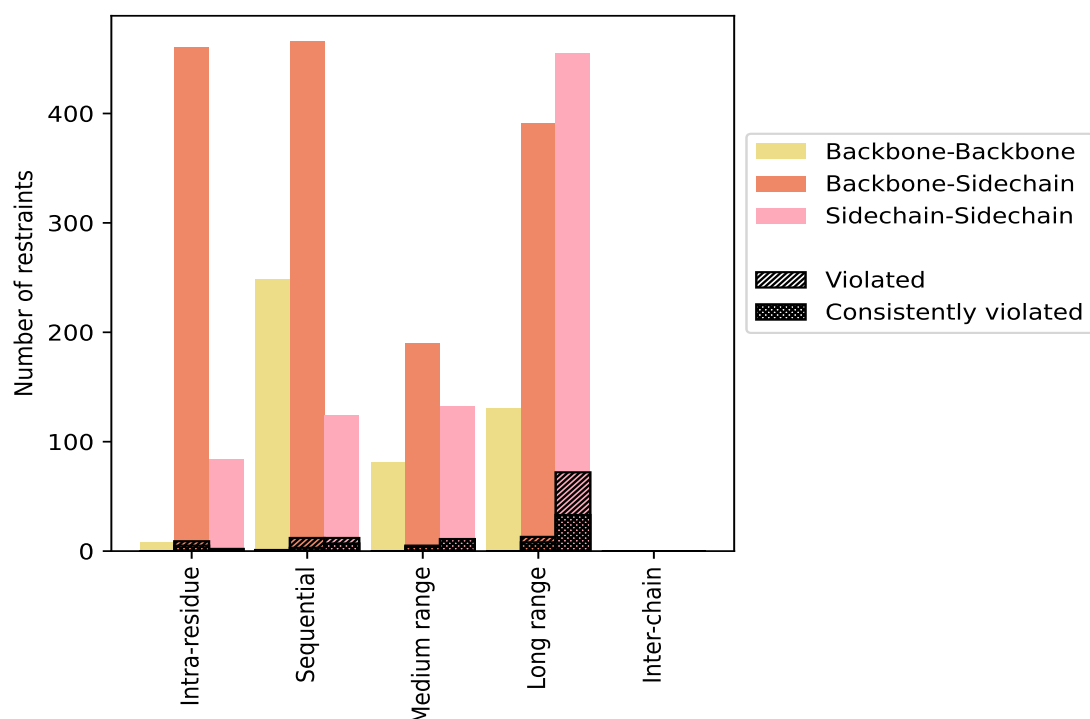
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>552</b>  | <b>19.9</b>    | <b>11</b>             | <b>2.0</b>     | <b>0.4</b>     | <b>5</b>                           | <b>0.9</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 8           | 0.3            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 460         | 16.6           | 9                     | 2.0            | 0.3            | 5                                  | 1.1            | 0.2            |
| Sidechain-Sidechain                                                         | 84          | 3.0            | 2                     | 2.4            | 0.1            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>838</b>  | <b>30.3</b>    | <b>25</b>             | <b>3.0</b>     | <b>0.9</b>     | <b>10</b>                          | <b>1.2</b>     | <b>0.4</b>     |
| Backbone-Backbone                                                           | 248         | 9.0            | 1                     | 0.4            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 466         | 16.8           | 12                    | 2.6            | 0.4            | 3                                  | 0.6            | 0.1            |
| Sidechain-Sidechain                                                         | 124         | 4.5            | 12                    | 9.7            | 0.4            | 7                                  | 5.6            | 0.3            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>403</b>  | <b>14.6</b>    | <b>16</b>             | <b>4.0</b>     | <b>0.6</b>     | <b>15</b>                          | <b>3.7</b>     | <b>0.5</b>     |
| Backbone-Backbone                                                           | 81          | 2.9            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 190         | 6.9            | 5                     | 2.6            | 0.2            | 4                                  | 2.1            | 0.1            |
| Sidechain-Sidechain                                                         | 132         | 4.8            | 11                    | 8.3            | 0.4            | 11                                 | 8.3            | 0.4            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>976</b>  | <b>35.2</b>    | <b>85</b>             | <b>8.7</b>     | <b>3.1</b>     | <b>41</b>                          | <b>4.2</b>     | <b>1.5</b>     |
| Backbone-Backbone                                                           | 130         | 4.7            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 391         | 14.1           | 13                    | 3.3            | 0.5            | 8                                  | 2.0            | 0.3            |
| Sidechain-Sidechain                                                         | 455         | 16.4           | 72                    | 15.8           | 2.6            | 33                                 | 7.3            | 1.2            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>2769</b> | <b>100.0</b>   | <b>137</b>            | <b>4.9</b>     | <b>4.9</b>     | <b>71</b>                          | <b>2.6</b>     | <b>2.6</b>     |
| Backbone-Backbone                                                           | 467         | 16.9           | 1                     | 0.2            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 1507        | 54.4           | 39                    | 2.6            | 1.4            | 20                                 | 1.3            | 0.7            |
| Sidechain-Sidechain                                                         | 795         | 28.7           | 97                    | 12.2           | 3.5            | 51                                 | 6.4            | 1.8            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 8                    | 18              | 15              | 55              | 0               | 96    | 1.91     | 4.14    | 1.07                | 1.85       |
| 2        | 7                    | 12              | 15              | 42              | 0               | 76    | 2.05     | 4.07    | 1.02                | 2.08       |
| 3        | 5                    | 10              | 15              | 45              | 0               | 75    | 2.02     | 4.09    | 1.06                | 2.01       |
| 4        | 8                    | 14              | 15              | 44              | 0               | 81    | 2.05     | 4.24    | 1.13                | 1.93       |
| 5        | 6                    | 12              | 15              | 43              | 0               | 76    | 2.14     | 4.12    | 1.07                | 2.25       |
| 6        | 6                    | 11              | 15              | 43              | 0               | 75    | 2.15     | 4.14    | 1.06                | 2.23       |
| 7        | 7                    | 18              | 15              | 51              | 0               | 91    | 1.97     | 4.15    | 1.06                | 1.93       |
| 8        | 7                    | 15              | 15              | 46              | 0               | 83    | 1.97     | 4.12    | 1.11                | 1.92       |
| 9        | 8                    | 14              | 15              | 46              | 0               | 83    | 1.94     | 4.25    | 1.12                | 1.94       |
| 10       | 8                    | 13              | 15              | 42              | 0               | 78    | 1.96     | 4.15    | 1.07                | 1.96       |

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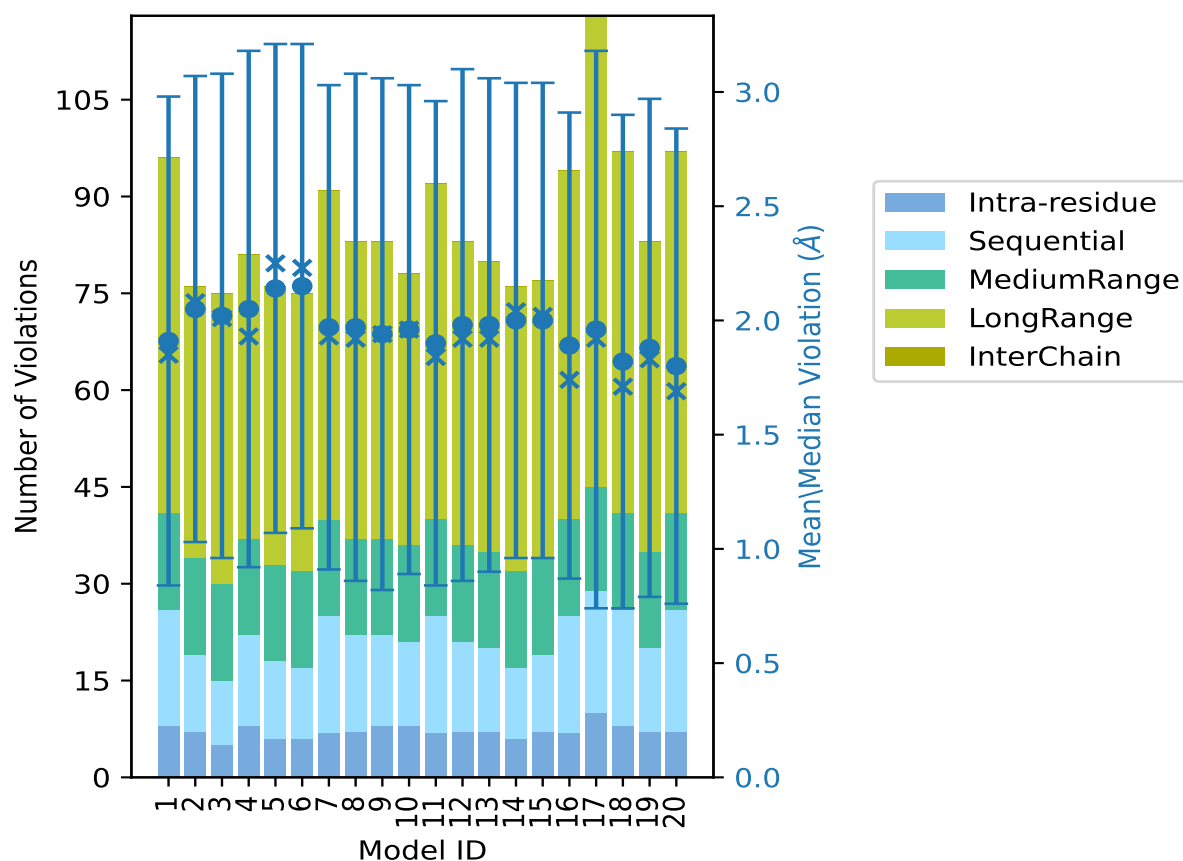
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 7                    | 18              | 15              | 52              | 0               | 92    | 1.9      | 4.07    | 1.06                | 1.84       |
| 12       | 7                    | 14              | 15              | 47              | 0               | 83    | 1.98     | 4.13    | 1.12                | 1.92       |
| 13       | 7                    | 13              | 15              | 45              | 0               | 80    | 1.98     | 4.24    | 1.08                | 1.92       |
| 14       | 6                    | 11              | 15              | 44              | 0               | 76    | 2.0      | 4.2     | 1.04                | 2.04       |
| 15       | 7                    | 12              | 15              | 43              | 0               | 77    | 2.0      | 4.2     | 1.04                | 2.02       |
| 16       | 7                    | 18              | 15              | 54              | 0               | 94    | 1.89     | 4.09    | 1.02                | 1.74       |
| 17       | 10                   | 19              | 16              | 73              | 0               | 118   | 1.96     | 6.88    | 1.22                | 1.92       |
| 18       | 8                    | 18              | 15              | 56              | 0               | 97    | 1.82     | 4.1     | 1.08                | 1.71       |
| 19       | 7                    | 13              | 15              | 48              | 0               | 83    | 1.88     | 4.08    | 1.09                | 1.83       |
| 20       | 7                    | 19              | 15              | 56              | 0               | 97    | 1.8      | 4.14    | 1.04                | 1.69       |

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

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

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



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

### 9.3 Distance violation statistics for the ensemble

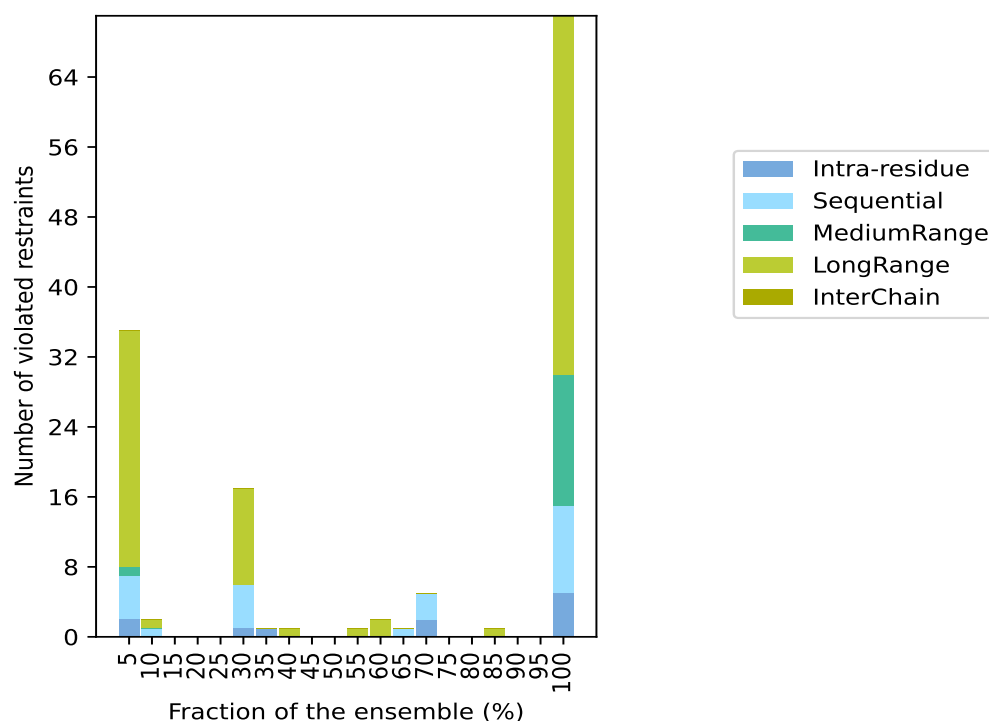
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2632(IR:541, SQ:813, MR:387, LR:891, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 2                             | 5               | 1               | 27              | 0               | 35    | 1                        | 5.0   |
| 0                             | 1               | 0               | 1               | 0               | 2     | 2                        | 10.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 3                        | 15.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 4                        | 20.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 5                        | 25.0  |
| 1                             | 5               | 0               | 11              | 0               | 17    | 6                        | 30.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 7                        | 35.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 8                        | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 9                        | 45.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 10                       | 50.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 11                       | 55.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 12                       | 60.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 13                       | 65.0  |
| 2                             | 3               | 0               | 0               | 0               | 5     | 14                       | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 15                       | 75.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 16                       | 80.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 17                       | 85.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 18                       | 90.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 19                       | 95.0  |
| 5                             | 10              | 15              | 41              | 0               | 71    | 20                       | 100.0 |

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

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

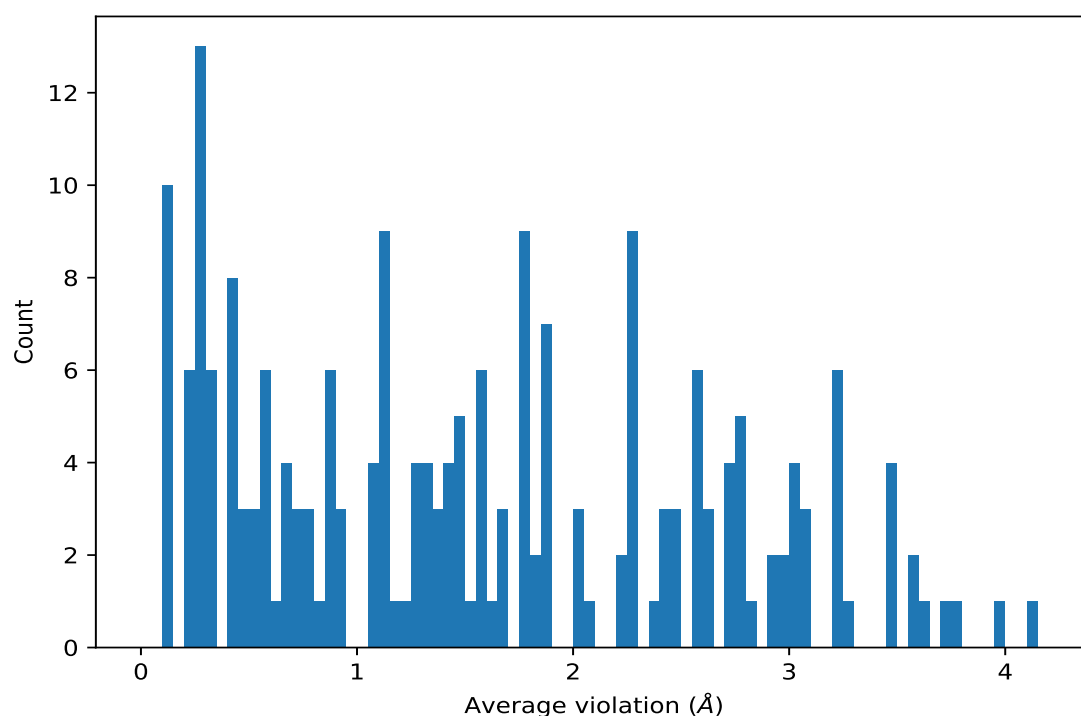
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 20                  | 4.14     | 0.06                | 4.14       |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 20                  | 3.99     | 0.02                | 3.99       |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 20                  | 3.8      | 0.02                | 3.8        |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 20                  | 3.7      | 0.06                | 3.7        |
| (1,1971) | 1:151:A:ASN:HA  | 1:161:A:PHE:HE2 | 20                  | 3.64     | 0.06                | 3.64       |
| (1,2474) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HZ  | 20                  | 3.56     | 0.07                | 3.58       |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 20                  | 3.56     | 0.76                | 3.4        |
| (1,110)  | 1:19:A:LEU:HG   | 1:22:A:PHE:HE1  | 20                  | 3.47     | 0.07                | 3.5        |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 20                  | 3.3      | 0.66                | 3.15       |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 20                  | 3.24     | 0.1                 | 3.23       |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 20                  | 3.24     | 0.1                 | 3.23       |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 20                  | 3.24     | 0.1                 | 3.23       |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 20                  | 3.2      | 0.1                 | 3.19       |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 20                  | 3.2      | 0.1                 | 3.19       |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 20                  | 3.2      | 0.1                 | 3.19       |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 20                  | 3.06     | 0.03                | 3.08       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2   | 20                  | 3.06     | 0.51                | 3.16       |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3   | 20                  | 3.06     | 0.51                | 3.16       |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ   | 20                  | 3.03     | 0.06                | 3.04       |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1   | 20                  | 3.02     | 0.19                | 3.0        |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1   | 20                  | 3.02     | 0.19                | 3.0        |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1   | 20                  | 3.02     | 0.19                | 3.0        |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2  | 20                  | 2.99     | 0.07                | 2.99       |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2  | 20                  | 2.95     | 1.12                | 3.06       |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2  | 20                  | 2.93     | 0.61                | 2.8        |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2  | 20                  | 2.92     | 0.78                | 2.78       |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1   | 20                  | 2.79     | 0.2                 | 2.8        |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1   | 20                  | 2.79     | 0.2                 | 2.8        |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1   | 20                  | 2.79     | 0.2                 | 2.8        |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2  | 20                  | 2.79     | 0.48                | 2.86       |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2   | 20                  | 2.79     | 0.08                | 2.8        |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1   | 20                  | 2.74     | 0.18                | 2.78       |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1   | 20                  | 2.74     | 0.18                | 2.78       |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1   | 20                  | 2.74     | 0.18                | 2.78       |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2   | 20                  | 2.74     | 0.08                | 2.74       |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2   | 20                  | 2.64     | 0.14                | 2.62       |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2   | 20                  | 2.64     | 0.14                | 2.62       |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2   | 20                  | 2.64     | 0.14                | 2.62       |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2  | 20                  | 2.58     | 0.08                | 2.56       |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2  | 20                  | 2.58     | 0.08                | 2.56       |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2  | 20                  | 2.58     | 0.08                | 2.56       |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1   | 20                  | 2.56     | 0.1                 | 2.59       |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2  | 20                  | 2.56     | 0.06                | 2.55       |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3  | 20                  | 2.56     | 0.06                | 2.55       |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 20                  | 2.49     | 0.03                | 2.49       |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 20                  | 2.49     | 0.03                | 2.49       |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 20                  | 2.49     | 0.03                | 2.49       |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 20                  | 2.42     | 0.06                | 2.43       |
| (1,1640) | 1:138:A:SER:HA  | 1:140:A:PHE:HD2  | 20                  | 2.42     | 0.82                | 2.07       |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2  | 20                  | 2.38     | 0.06                | 2.38       |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1   | 20                  | 2.3      | 0.24                | 2.25       |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2   | 20                  | 2.29     | 0.18                | 2.32       |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1   | 20                  | 2.28     | 0.13                | 2.33       |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1   | 20                  | 2.28     | 0.13                | 2.33       |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1   | 20                  | 2.28     | 0.13                | 2.33       |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1   | 20                  | 2.27     | 0.07                | 2.28       |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1   | 20                  | 2.27     | 0.07                | 2.28       |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1   | 20                  | 2.27     | 0.07                | 2.28       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1646) | 1:139:A:LEU:HB2  | 1:140:A:PHE:HD2 | 20                  | 2.27     | 0.27                | 2.36       |
| (1,107)  | 1:19:A:LEU:HB2   | 1:22:A:PHE:HE1  | 20                  | 2.23     | 0.05                | 2.25       |
| (1,107)  | 1:19:A:LEU:HB3   | 1:22:A:PHE:HE1  | 20                  | 2.23     | 0.05                | 2.25       |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2 | 20                  | 2.06     | 0.9                 | 1.94       |
| (1,963)  | 1:23:A:ALA:HB1   | 1:86:A:PHE:HD2  | 20                  | 2.03     | 0.12                | 1.98       |
| (1,963)  | 1:23:A:ALA:HB2   | 1:86:A:PHE:HD2  | 20                  | 2.03     | 0.12                | 1.98       |
| (1,963)  | 1:23:A:ALA:HB3   | 1:86:A:PHE:HD2  | 20                  | 2.03     | 0.12                | 1.98       |
| (1,109)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HE1  | 20                  | 1.9      | 0.06                | 1.92       |
| (1,109)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HE1  | 20                  | 1.9      | 0.06                | 1.92       |
| (1,109)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HE1  | 20                  | 1.9      | 0.06                | 1.92       |
| (1,2410) | 1:161:A:PHE:HD1  | 1:182:A:LYS:HG2 | 20                  | 1.89     | 0.03                | 1.88       |
| (1,2410) | 1:161:A:PHE:HD1  | 1:182:A:LYS:HG3 | 20                  | 1.89     | 0.03                | 1.88       |
| (1,112)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HE1  | 20                  | 1.86     | 0.12                | 1.9        |
| (1,970)  | 1:25:A:ASP:H     | 1:86:A:PHE:HE2  | 20                  | 1.83     | 0.21                | 1.86       |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2  | 20                  | 1.79     | 0.06                | 1.79       |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2 | 20                  | 1.77     | 0.04                | 1.78       |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3 | 20                  | 1.77     | 0.04                | 1.78       |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 20                  | 1.75     | 0.03                | 1.75       |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 20                  | 1.75     | 0.03                | 1.75       |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 20                  | 1.75     | 0.03                | 1.75       |
| (1,116)  | 1:21:A:ARG:HG2   | 1:22:A:PHE:HE2  | 20                  | 1.61     | 0.11                | 1.65       |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2 | 20                  | 1.5      | 0.35                | 1.48       |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 20                  | 1.49     | 0.14                | 1.5        |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1  | 20                  | 1.49     | 0.14                | 1.5        |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1  | 20                  | 1.49     | 0.14                | 1.5        |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 20                  | 1.47     | 0.07                | 1.48       |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 20                  | 1.47     | 0.07                | 1.48       |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1 | 20                  | 1.45     | 0.08                | 1.44       |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1 | 20                  | 1.45     | 0.08                | 1.44       |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1 | 20                  | 1.45     | 0.08                | 1.44       |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 20                  | 1.39     | 0.07                | 1.37       |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 20                  | 1.39     | 0.07                | 1.37       |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 20                  | 1.39     | 0.03                | 1.39       |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 20                  | 1.33     | 0.04                | 1.33       |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 20                  | 1.33     | 0.04                | 1.33       |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 20                  | 1.33     | 0.04                | 1.33       |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 20                  | 1.33     | 0.06                | 1.34       |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 20                  | 1.29     | 0.02                | 1.3        |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 20                  | 1.27     | 0.05                | 1.27       |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 20                  | 1.27     | 0.05                | 1.27       |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 20                  | 1.27     | 0.05                | 1.27       |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1  | 20                  | 1.22     | 0.2                 | 1.17       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2 | 20                  | 1.19     | 0.02                | 1.2        |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2  | 20                  | 1.12     | 0.09                | 1.14       |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2  | 20                  | 1.12     | 0.09                | 1.14       |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2  | 20                  | 1.12     | 0.09                | 1.14       |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1  | 20                  | 1.07     | 0.21                | 1.02       |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2 | 20                  | 1.06     | 0.06                | 1.06       |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2 | 20                  | 1.06     | 0.06                | 1.06       |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2 | 20                  | 1.06     | 0.06                | 1.06       |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1  | 20                  | 0.94     | 0.14                | 0.92       |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1  | 20                  | 0.94     | 0.14                | 0.92       |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2  | 20                  | 0.91     | 0.03                | 0.92       |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 20                  | 0.88     | 0.29                | 0.84       |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 20                  | 0.88     | 0.29                | 0.84       |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 20                  | 0.88     | 0.29                | 0.84       |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 20                  | 0.88     | 0.29                | 0.84       |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 20                  | 0.88     | 0.29                | 0.84       |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 20                  | 0.88     | 0.29                | 0.84       |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 20                  | 0.68     | 0.08                | 0.7        |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 20                  | 0.68     | 0.08                | 0.7        |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 20                  | 0.68     | 0.08                | 0.7        |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2  | 20                  | 0.67     | 0.06                | 0.65       |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 20                  | 0.58     | 0.16                | 0.54       |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 20                  | 0.58     | 0.16                | 0.54       |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 20                  | 0.58     | 0.16                | 0.54       |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 20                  | 0.58     | 0.16                | 0.54       |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 20                  | 0.58     | 0.16                | 0.54       |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 20                  | 0.58     | 0.16                | 0.54       |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 20                  | 0.44     | 0.07                | 0.44       |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 20                  | 0.44     | 0.07                | 0.44       |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 20                  | 0.41     | 0.16                | 0.39       |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 20                  | 0.41     | 0.16                | 0.39       |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 20                  | 0.41     | 0.16                | 0.39       |
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 17                  | 0.2      | 0.07                | 0.19       |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 17                  | 0.2      | 0.07                | 0.19       |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 17                  | 0.2      | 0.07                | 0.19       |
| (1,1055) | 1:94:A:SER:HA    | 1:95:A:PHE:HE2  | 14                  | 1.83     | 0.78                | 2.14       |
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 14                  | 0.48     | 0.14                | 0.39       |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 14                  | 0.14     | 0.01                | 0.14       |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 14                  | 0.12     | 0.0                 | 0.12       |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB2  | 14                  | 0.11     | 0.01                | 0.11       |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB3  | 14                  | 0.11     | 0.01                | 0.11       |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 13                  | 0.33     | 0.13                | 0.37       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2  | 13                  | 0.33     | 0.13                | 0.37       |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2  | 13                  | 0.33     | 0.13                | 0.37       |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2  | 13                  | 0.33     | 0.13                | 0.37       |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2  | 13                  | 0.33     | 0.13                | 0.37       |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2  | 13                  | 0.33     | 0.13                | 0.37       |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1   | 12                  | 0.51     | 0.18                | 0.58       |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1   | 12                  | 0.51     | 0.18                | 0.58       |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1   | 12                  | 0.51     | 0.18                | 0.58       |
| (1,965)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HE1   | 12                  | 0.44     | 0.18                | 0.49       |
| (1,965)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HE1   | 12                  | 0.44     | 0.18                | 0.49       |
| (1,965)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HE1   | 12                  | 0.44     | 0.18                | 0.49       |
| (1,663)  | 1:36:A:GLU:HG2   | 1:60:A:LEU:HG    | 11                  | 0.1      | 0.0                 | 0.1        |
| (1,663)  | 1:36:A:GLU:HG3   | 1:60:A:LEU:HG    | 11                  | 0.1      | 0.0                 | 0.1        |
| (1,969)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1   | 8                   | 0.29     | 0.08                | 0.28       |
| (1,969)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1   | 8                   | 0.29     | 0.08                | 0.28       |
| (1,969)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1   | 8                   | 0.29     | 0.08                | 0.28       |
| (1,969)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1   | 8                   | 0.29     | 0.08                | 0.28       |
| (1,969)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1   | 8                   | 0.29     | 0.08                | 0.28       |
| (1,969)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1   | 8                   | 0.29     | 0.08                | 0.28       |
| (1,811)  | 1:71:A:LYS:HA    | 1:71:A:LYS:HG2   | 7                   | 0.11     | 0.02                | 0.11       |
| (1,811)  | 1:71:A:LYS:HA    | 1:71:A:LYS:HG3   | 7                   | 0.11     | 0.02                | 0.11       |
| (1,1667) | 1:129:A:ILE:HD11 | 1:142:A:TYR:HD1  | 6                   | 3.47     | 0.13                | 3.52       |
| (1,1667) | 1:129:A:ILE:HD12 | 1:142:A:TYR:HD1  | 6                   | 3.47     | 0.13                | 3.52       |
| (1,1667) | 1:129:A:ILE:HD13 | 1:142:A:TYR:HD1  | 6                   | 3.47     | 0.13                | 3.52       |
| (1,1676) | 1:141:A:PRO:HB3  | 1:142:A:TYR:HE2  | 6                   | 2.83     | 0.22                | 2.78       |
| (1,1678) | 1:141:A:PRO:HA   | 1:142:A:TYR:HD2  | 6                   | 2.44     | 0.09                | 2.44       |
| (1,1689) | 1:142:A:TYR:HD1  | 1:143:A:GLU:H    | 6                   | 1.87     | 0.03                | 1.87       |
| (1,2101) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG11 | 6                   | 1.78     | 0.12                | 1.81       |
| (1,2101) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG12 | 6                   | 1.78     | 0.12                | 1.81       |
| (1,2101) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG13 | 6                   | 1.78     | 0.12                | 1.81       |
| (1,1668) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HD1  | 6                   | 1.66     | 0.12                | 1.66       |
| (1,1668) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HD1  | 6                   | 1.66     | 0.12                | 1.66       |
| (1,1668) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HD1  | 6                   | 1.66     | 0.12                | 1.66       |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG11 | 6                   | 1.57     | 0.16                | 1.54       |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG12 | 6                   | 1.57     | 0.16                | 1.54       |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG13 | 6                   | 1.57     | 0.16                | 1.54       |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG21 | 6                   | 1.57     | 0.16                | 1.54       |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG22 | 6                   | 1.57     | 0.16                | 1.54       |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG23 | 6                   | 1.57     | 0.16                | 1.54       |
| (1,2103) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HB   | 6                   | 1.42     | 0.22                | 1.44       |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD11 | 6                   | 1.11     | 0.19                | 1.11       |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD12 | 6                   | 1.11     | 0.19                | 1.11       |

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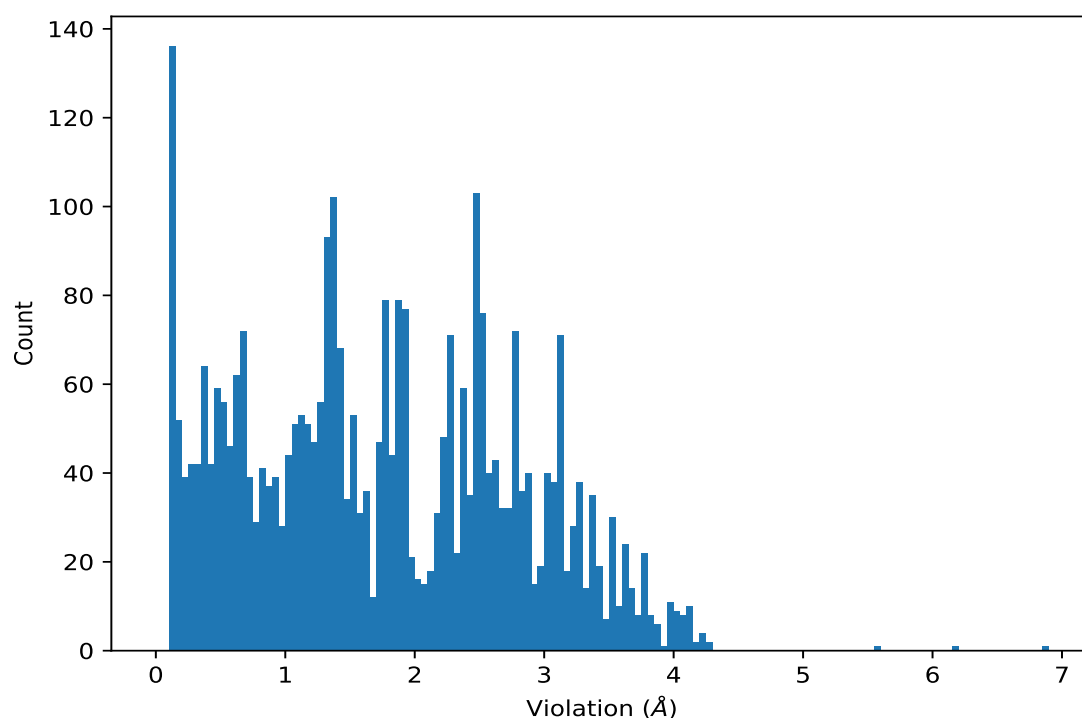
| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD13 | 6                   | 1.11     | 0.19                | 1.11       |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD21 | 6                   | 1.11     | 0.19                | 1.11       |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD22 | 6                   | 1.11     | 0.19                | 1.11       |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD23 | 6                   | 1.11     | 0.19                | 1.11       |
| (1,1675) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HE2  | 6                   | 0.8      | 0.32                | 0.68       |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG21 | 6                   | 0.77     | 0.13                | 0.8        |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG22 | 6                   | 0.77     | 0.13                | 0.8        |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG23 | 6                   | 0.77     | 0.13                | 0.8        |
| (1,1666) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HE1  | 6                   | 0.73     | 0.15                | 0.7        |
| (1,1666) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HE1  | 6                   | 0.73     | 0.15                | 0.7        |
| (1,1666) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HE1  | 6                   | 0.73     | 0.15                | 0.7        |
| (1,1677) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HD2  | 6                   | 0.64     | 0.25                | 0.56       |
| (1,2104) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HB   | 6                   | 0.49     | 0.09                | 0.47       |
| (1,1687) | 1:142:A:TYR:HB3  | 1:142:A:TYR:HD2  | 6                   | 0.48     | 0.02                | 0.48       |
| (1,973)  | 1:27:A:HIS:HD2   | 1:86:A:PHE:HD2   | 6                   | 0.25     | 0.16                | 0.15       |
| (1,968)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1   | 6                   | 0.21     | 0.07                | 0.2        |
| (1,968)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1   | 6                   | 0.21     | 0.07                | 0.2        |
| (1,968)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1   | 6                   | 0.21     | 0.07                | 0.2        |
| (1,1054) | 1:89:A:VAL:HG11  | 1:95:A:PHE:HD2   | 2                   | 0.29     | 0.18                | 0.29       |
| (1,1054) | 1:89:A:VAL:HG12  | 1:95:A:PHE:HD2   | 2                   | 0.29     | 0.18                | 0.29       |
| (1,1054) | 1:89:A:VAL:HG13  | 1:95:A:PHE:HD2   | 2                   | 0.29     | 0.18                | 0.29       |
| (1,1054) | 1:89:A:VAL:HG21  | 1:95:A:PHE:HD2   | 2                   | 0.29     | 0.18                | 0.29       |
| (1,1054) | 1:89:A:VAL:HG22  | 1:95:A:PHE:HD2   | 2                   | 0.29     | 0.18                | 0.29       |
| (1,1054) | 1:89:A:VAL:HG23  | 1:95:A:PHE:HD2   | 2                   | 0.29     | 0.18                | 0.29       |
| (1,47)   | 1:14:A:PRO:HB2   | 1:15:A:ASP:H     | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,47)   | 1:14:A:PRO:HB3   | 1:15:A:ASP:H     | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 17       | 6.88          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 17       | 6.18          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 17       | 5.6           |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 9        | 4.25          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 17       | 4.25          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 4        | 4.24          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 13       | 4.24          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 14       | 4.2           |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 15       | 4.2           |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 7        | 4.15          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 10       | 4.15          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 1        | 4.14          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 6        | 4.14          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 20       | 4.14          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 9        | 4.14          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 6        | 4.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 12       | 4.13          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 4        | 4.12          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 5        | 4.12          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 8        | 4.12          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 5        | 4.11          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 18       | 4.1           |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 3        | 4.09          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 12       | 4.09          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 16       | 4.09          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 19       | 4.08          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 2        | 4.07          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 8        | 4.07          |
| (1,2406) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HD3 | 11       | 4.07          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 11       | 4.03          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 3        | 4.02          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 7        | 4.02          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 19       | 4.02          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 12       | 4.01          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 8        | 4.0           |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 17       | 4.0           |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 18       | 4.0           |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 20       | 4.0           |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 2        | 3.99          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 10       | 3.99          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 9        | 3.98          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 1        | 3.97          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 4        | 3.97          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 5        | 3.97          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 13       | 3.97          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 15       | 3.97          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 16       | 3.97          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 7        | 3.97          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 14       | 3.95          |
| (1,2407) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HA  | 6        | 3.94          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 9        | 3.89          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 4        | 3.86          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 5        | 3.86          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 12       | 3.86          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 8        | 3.85          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 6        | 3.85          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 17       | 3.84          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 20       | 3.84          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 8        | 3.84          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 7        | 3.83          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 12       | 3.83          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 19       | 3.82          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 5        | 3.81          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 2        | 3.81          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 3        | 3.8           |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 9        | 3.8           |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 10       | 3.8           |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 11       | 3.8           |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 1        | 3.79          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 2        | 3.79          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 15       | 3.79          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 16       | 3.79          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 18       | 3.79          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 16       | 3.79          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 18       | 3.79          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 5        | 3.79          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 5        | 3.79          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 4        | 3.78          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 13       | 3.78          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 6        | 3.77          |
| (1,2405) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HA  | 14       | 3.77          |
| (1,1971) | 1:151:A:ASN:HA  | 1:161:A:PHE:HE2 | 2        | 3.76          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 6        | 3.76          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 6        | 3.76          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 6        | 3.75          |
| (1,1971) | 1:151:A:ASN:HA  | 1:161:A:PHE:HE2 | 16       | 3.75          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 4        | 3.74          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 11       | 3.74          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 3        | 3.73          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 13       | 3.73          |
| (1,1971) | 1:151:A:ASN:HA  | 1:161:A:PHE:HE2 | 18       | 3.72          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 1        | 3.71          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 14       | 3.7           |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 19       | 3.7           |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 5        | 3.69          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 17       | 3.69          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 2        | 3.69          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 2        | 3.69          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 9        | 3.68          |
| (1,1972) | 1:152:A:ALA:H   | 1:161:A:PHE:HE2 | 10       | 3.68          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1972) | 1:152:A:ALA:H    | 1:161:A:PHE:HE2 | 15       | 3.68          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 17       | 3.68          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 14       | 3.67          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 6        | 3.67          |
| (1,870)  | 1:22:A:PHE:HE1   | 1:81:A:LYS:HE2  | 3        | 3.67          |
| (1,870)  | 1:22:A:PHE:HE1   | 1:81:A:LYS:HE3  | 3        | 3.67          |
| (1,1972) | 1:152:A:ALA:H    | 1:161:A:PHE:HE2 | 12       | 3.66          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 5        | 3.66          |
| (1,1972) | 1:152:A:ALA:H    | 1:161:A:PHE:HE2 | 7        | 3.65          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 11       | 3.65          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 15       | 3.64          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 3        | 3.64          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 4        | 3.64          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 19       | 3.64          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 4        | 3.63          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 6        | 3.63          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 1        | 3.63          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 13       | 3.63          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 14       | 3.63          |
| (1,1638) | 1:138:A:SER:HB2  | 1:140:A:PHE:HE2 | 7        | 3.63          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 1        | 3.62          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 9        | 3.62          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 9        | 3.62          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 10       | 3.62          |
| (1,1639) | 1:138:A:SER:HB3  | 1:140:A:PHE:HE2 | 13       | 3.62          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 7        | 3.61          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 13       | 3.6           |
| (1,1972) | 1:152:A:ALA:H    | 1:161:A:PHE:HE2 | 20       | 3.6           |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 12       | 3.6           |
| (1,1667) | 1:129:A:ILE:HD11 | 1:142:A:TYR:HD1 | 18       | 3.6           |
| (1,1667) | 1:129:A:ILE:HD12 | 1:142:A:TYR:HD1 | 18       | 3.6           |
| (1,1667) | 1:129:A:ILE:HD13 | 1:142:A:TYR:HD1 | 18       | 3.6           |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 18       | 3.59          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 15       | 3.59          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 10       | 3.58          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 16       | 3.58          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 12       | 3.57          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 19       | 3.57          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 20       | 3.57          |
| (1,1667) | 1:129:A:ILE:HD11 | 1:142:A:TYR:HD1 | 20       | 3.57          |
| (1,1667) | 1:129:A:ILE:HD12 | 1:142:A:TYR:HD1 | 20       | 3.57          |
| (1,1667) | 1:129:A:ILE:HD13 | 1:142:A:TYR:HD1 | 20       | 3.57          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 2        | 3.55          |
| (1,1640) | 1:138:A:SER:HA   | 1:140:A:PHE:HD2 | 6        | 3.55          |
| (1,1640) | 1:138:A:SER:HA   | 1:140:A:PHE:HD2 | 12       | 3.55          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 14       | 3.55          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 11       | 3.54          |
| (1,1667) | 1:129:A:ILE:HD11 | 1:142:A:TYR:HD1 | 7        | 3.54          |
| (1,1667) | 1:129:A:ILE:HD12 | 1:142:A:TYR:HD1 | 7        | 3.54          |
| (1,1667) | 1:129:A:ILE:HD13 | 1:142:A:TYR:HD1 | 7        | 3.54          |
| (1,1640) | 1:138:A:SER:HA   | 1:140:A:PHE:HD2 | 5        | 3.54          |
| (1,1640) | 1:138:A:SER:HA   | 1:140:A:PHE:HD2 | 8        | 3.54          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 15       | 3.54          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 3        | 3.53          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 5        | 3.53          |
| (1,1640) | 1:138:A:SER:HA   | 1:140:A:PHE:HD2 | 4        | 3.53          |
| (1,1639) | 1:138:A:SER:HB3  | 1:140:A:PHE:HE2 | 1        | 3.53          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 10       | 3.53          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 20       | 3.52          |
| (1,1972) | 1:152:A:ALA:H    | 1:161:A:PHE:HE2 | 8        | 3.52          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 6        | 3.52          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 11       | 3.52          |
| (1,1971) | 1:151:A:ASN:HA   | 1:161:A:PHE:HE2 | 8        | 3.51          |
| (1,1667) | 1:129:A:ILE:HD11 | 1:142:A:TYR:HD1 | 1        | 3.51          |
| (1,1667) | 1:129:A:ILE:HD12 | 1:142:A:TYR:HD1 | 1        | 3.51          |
| (1,1667) | 1:129:A:ILE:HD13 | 1:142:A:TYR:HD1 | 1        | 3.51          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 2        | 3.51          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 3        | 3.51          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 5        | 3.51          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 13       | 3.51          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 18       | 3.51          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 7        | 3.5           |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 1        | 3.49          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 4        | 3.49          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 16       | 3.49          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 7        | 3.47          |
| (1,2474) | 1:161:A:PHE:HE1  | 1:189:A:PHE:HZ  | 8        | 3.45          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 8        | 3.45          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 17       | 3.45          |
| (1,870)  | 1:22:A:PHE:HE1   | 1:81:A:LYS:HE2  | 19       | 3.44          |
| (1,870)  | 1:22:A:PHE:HE1   | 1:81:A:LYS:HE3  | 19       | 3.44          |
| (1,2478) | 1:161:A:PHE:HD1  | 1:189:A:PHE:HE2 | 11       | 3.43          |
| (1,2478) | 1:161:A:PHE:HD1  | 1:189:A:PHE:HE2 | 18       | 3.43          |
| (1,2473) | 1:161:A:PHE:HB3  | 1:189:A:PHE:HE2 | 17       | 3.43          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 11       | 3.43          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 11       | 3.43          |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 3        | 3.42          |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 4        | 3.42          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 20       | 3.42          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 20       | 3.42          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 20       | 3.42          |
| (1,110)  | 1:19:A:LEU:HG   | 1:22:A:PHE:HE1  | 19       | 3.42          |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 2        | 3.41          |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 14       | 3.41          |
| (1,2474) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HZ  | 17       | 3.41          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 8        | 3.41          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 8        | 3.41          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 8        | 3.41          |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 9        | 3.4           |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 13       | 3.4           |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 15       | 3.4           |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 12       | 3.4           |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 12       | 3.4           |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 12       | 3.4           |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 1        | 3.39          |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 6        | 3.39          |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 10       | 3.39          |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 12       | 3.39          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 12       | 3.39          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 12       | 3.39          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 12       | 3.39          |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 19       | 3.38          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 20       | 3.38          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 20       | 3.38          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 20       | 3.38          |
| (1,2478) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HE2 | 16       | 3.37          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 1        | 3.37          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 8        | 3.37          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 8        | 3.37          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 8        | 3.37          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 13       | 3.37          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 13       | 3.37          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 18       | 3.37          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 18       | 3.37          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 12       | 3.36          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 12       | 3.36          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,981)  | 1:35:A:LEU:HD23  | 1:86:A:PHE:HD1  | 12       | 3.36          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 9        | 3.36          |
| (1,2478) | 1:161:A:PHE:HD1  | 1:189:A:PHE:HE2 | 7        | 3.35          |
| (1,979)  | 1:35:A:LEU:HD21  | 1:86:A:PHE:HD1  | 1        | 3.35          |
| (1,979)  | 1:35:A:LEU:HD22  | 1:86:A:PHE:HD1  | 1        | 3.35          |
| (1,979)  | 1:35:A:LEU:HD23  | 1:86:A:PHE:HD1  | 1        | 3.35          |
| (1,110)  | 1:19:A:LEU:HG    | 1:22:A:PHE:HE1  | 12       | 3.35          |
| (1,977)  | 1:35:A:LEU:HD21  | 1:86:A:PHE:HE1  | 20       | 3.34          |
| (1,977)  | 1:35:A:LEU:HD22  | 1:86:A:PHE:HE1  | 20       | 3.34          |
| (1,977)  | 1:35:A:LEU:HD23  | 1:86:A:PHE:HE1  | 20       | 3.34          |
| (1,2478) | 1:161:A:PHE:HD1  | 1:189:A:PHE:HE2 | 5        | 3.33          |
| (1,2478) | 1:161:A:PHE:HD1  | 1:189:A:PHE:HE2 | 20       | 3.33          |
| (1,979)  | 1:35:A:LEU:HD21  | 1:86:A:PHE:HD1  | 18       | 3.32          |
| (1,979)  | 1:35:A:LEU:HD22  | 1:86:A:PHE:HD1  | 18       | 3.32          |
| (1,979)  | 1:35:A:LEU:HD23  | 1:86:A:PHE:HD1  | 18       | 3.32          |
| (1,981)  | 1:35:A:LEU:HD21  | 1:86:A:PHE:HD1  | 1        | 3.31          |
| (1,981)  | 1:35:A:LEU:HD22  | 1:86:A:PHE:HD1  | 1        | 3.31          |
| (1,981)  | 1:35:A:LEU:HD23  | 1:86:A:PHE:HD1  | 1        | 3.31          |
| (1,979)  | 1:35:A:LEU:HD21  | 1:86:A:PHE:HD1  | 19       | 3.31          |
| (1,979)  | 1:35:A:LEU:HD22  | 1:86:A:PHE:HD1  | 19       | 3.31          |
| (1,979)  | 1:35:A:LEU:HD23  | 1:86:A:PHE:HD1  | 19       | 3.31          |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2 | 6        | 3.3           |
| (1,977)  | 1:35:A:LEU:HD21  | 1:86:A:PHE:HE1  | 8        | 3.3           |
| (1,977)  | 1:35:A:LEU:HD22  | 1:86:A:PHE:HE1  | 8        | 3.3           |
| (1,977)  | 1:35:A:LEU:HD23  | 1:86:A:PHE:HE1  | 8        | 3.3           |
| (1,1667) | 1:129:A:ILE:HD11 | 1:142:A:TYR:HD1 | 16       | 3.29          |
| (1,1667) | 1:129:A:ILE:HD12 | 1:142:A:TYR:HD1 | 16       | 3.29          |
| (1,1667) | 1:129:A:ILE:HD13 | 1:142:A:TYR:HD1 | 16       | 3.29          |
| (1,870)  | 1:22:A:PHE:HE1   | 1:81:A:LYS:HE2  | 4        | 3.29          |
| (1,870)  | 1:22:A:PHE:HE1   | 1:81:A:LYS:HE3  | 4        | 3.29          |
| (1,2478) | 1:161:A:PHE:HD1  | 1:189:A:PHE:HE2 | 8        | 3.28          |
| (1,1667) | 1:129:A:ILE:HD11 | 1:142:A:TYR:HD1 | 11       | 3.28          |
| (1,1667) | 1:129:A:ILE:HD12 | 1:142:A:TYR:HD1 | 11       | 3.28          |
| (1,1667) | 1:129:A:ILE:HD13 | 1:142:A:TYR:HD1 | 11       | 3.28          |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2 | 12       | 3.28          |
| (1,981)  | 1:35:A:LEU:HD21  | 1:86:A:PHE:HD1  | 18       | 3.28          |
| (1,981)  | 1:35:A:LEU:HD22  | 1:86:A:PHE:HD1  | 18       | 3.28          |
| (1,981)  | 1:35:A:LEU:HD23  | 1:86:A:PHE:HD1  | 18       | 3.28          |
| (1,979)  | 1:35:A:LEU:HD21  | 1:86:A:PHE:HD1  | 4        | 3.28          |
| (1,979)  | 1:35:A:LEU:HD22  | 1:86:A:PHE:HD1  | 4        | 3.28          |
| (1,979)  | 1:35:A:LEU:HD23  | 1:86:A:PHE:HD1  | 4        | 3.28          |
| (1,979)  | 1:35:A:LEU:HD21  | 1:86:A:PHE:HD1  | 17       | 3.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 17       | 3.28          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 17       | 3.28          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 1        | 3.28          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 1        | 3.28          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 1        | 3.28          |
| (1,1641) | 1:138:A:SER:HA  | 1:140:A:PHE:HE2 | 5        | 3.27          |
| (1,1641) | 1:138:A:SER:HA  | 1:140:A:PHE:HE2 | 8        | 3.27          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 19       | 3.27          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 19       | 3.27          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 19       | 3.27          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 9        | 3.27          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 9        | 3.27          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 9        | 3.27          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 2        | 3.26          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 13       | 3.26          |
| (1,1641) | 1:138:A:SER:HA  | 1:140:A:PHE:HE2 | 4        | 3.26          |
| (1,110)  | 1:19:A:LEU:HG   | 1:22:A:PHE:HE1  | 20       | 3.26          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 11       | 3.24          |
| (1,1640) | 1:138:A:SER:HA  | 1:140:A:PHE:HD2 | 7        | 3.24          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 4        | 3.24          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 4        | 3.24          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 4        | 3.24          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 17       | 3.24          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 17       | 3.24          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 17       | 3.24          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 16       | 3.24          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 16       | 3.24          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 16       | 3.24          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 3        | 3.23          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 9        | 3.23          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 9        | 3.23          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 9        | 3.23          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 13       | 3.22          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 13       | 3.22          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 13       | 3.22          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 2        | 3.21          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 18       | 3.21          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 11       | 3.2           |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 15       | 3.2           |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 17       | 3.2           |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 16       | 3.2           |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 16       | 3.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 16       | 3.2           |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 14       | 3.2           |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 14       | 3.2           |
| (1,1676) | 1:141:A:PRO:HB3 | 1:142:A:TYR:HE2 | 20       | 3.19          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 15       | 3.19          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 5        | 3.19          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 5        | 3.19          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 5        | 3.19          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 13       | 3.18          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 13       | 3.18          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 13       | 3.18          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 4        | 3.17          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 14       | 3.17          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 6        | 3.17          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 6        | 3.17          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 6        | 3.17          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 7        | 3.16          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 13       | 3.16          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 4        | 3.16          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 4        | 3.16          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 4        | 3.16          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 10       | 3.15          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 12       | 3.15          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 19       | 3.15          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 5        | 3.15          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 5        | 3.15          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 5        | 3.15          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 14       | 3.15          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 14       | 3.15          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 14       | 3.15          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 16       | 3.14          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 11       | 3.14          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 11       | 3.14          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 11       | 3.14          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 15       | 3.14          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 15       | 3.14          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 15       | 3.14          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 1        | 3.13          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 6        | 3.13          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 14       | 3.13          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 16       | 3.13          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 1        | 3.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 1        | 3.13          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 1        | 3.13          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 6        | 3.13          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 6        | 3.13          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 6        | 3.13          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 3        | 3.13          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 3        | 3.13          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 3        | 3.13          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 10       | 3.13          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 10       | 3.13          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 10       | 3.13          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 14       | 3.12          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 9        | 3.12          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 15       | 3.12          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 2        | 3.12          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 16       | 3.12          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 16       | 3.12          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 16       | 3.12          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 17       | 3.12          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 17       | 3.12          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 17       | 3.12          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 17       | 3.12          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 17       | 3.12          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 17       | 3.12          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 15       | 3.12          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 15       | 3.12          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 5        | 3.11          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 20       | 3.11          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 14       | 3.11          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 14       | 3.11          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 14       | 3.11          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 18       | 3.11          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 18       | 3.11          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 18       | 3.11          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 3        | 3.1           |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 4        | 3.1           |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 11       | 3.1           |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 13       | 3.1           |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 17       | 3.1           |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 19       | 3.1           |
| (1,1055) | 1:94:A:SER:HA   | 1:95:A:PHE:HE2  | 10       | 3.1           |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 11       | 3.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 11       | 3.1           |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 11       | 3.1           |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 15       | 3.1           |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 15       | 3.1           |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 15       | 3.1           |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 7        | 3.1           |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 7        | 3.1           |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 7        | 3.1           |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 4        | 3.09          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 6        | 3.09          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 15       | 3.09          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 1        | 3.09          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 14       | 3.09          |
| (1,1640) | 1:138:A:SER:HA  | 1:140:A:PHE:HD2 | 9        | 3.09          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 3        | 3.09          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 3        | 3.09          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 3        | 3.09          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 10       | 3.09          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 10       | 3.09          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 10       | 3.09          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 9        | 3.08          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 9        | 3.08          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 10       | 3.08          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 12       | 3.08          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 15       | 3.08          |
| (1,979)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 2        | 3.08          |
| (1,979)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 2        | 3.08          |
| (1,979)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 2        | 3.08          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 1        | 3.07          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 13       | 3.07          |
| (1,2475) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HD2 | 8        | 3.07          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 6        | 3.07          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 7        | 3.07          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 4        | 3.07          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 4        | 3.07          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 4        | 3.07          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 19       | 3.07          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 19       | 3.07          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 19       | 3.07          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 10       | 3.07          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 10       | 3.07          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 18       | 3.06          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 18       | 3.06          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 7        | 3.06          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 7        | 3.06          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 7        | 3.06          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 8        | 3.05          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 19       | 3.05          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 13       | 3.05          |
| (1,2573) | 1:189:A:PHE:HD2 | 1:191:A:LEU:HA  | 17       | 3.04          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 12       | 3.04          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 16       | 3.04          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 2        | 3.04          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 1        | 3.04          |
| (1,1676) | 1:141:A:PRO:HB3 | 1:142:A:TYR:HE2 | 16       | 3.04          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 18       | 3.04          |
| (1,981)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HD1  | 2        | 3.04          |
| (1,981)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HD1  | 2        | 3.04          |
| (1,981)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HD1  | 2        | 3.04          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 16       | 3.04          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 16       | 3.04          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 16       | 3.04          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 10       | 3.03          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 19       | 3.03          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 20       | 3.03          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 5        | 3.03          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 11       | 3.03          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 9        | 3.03          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 9        | 3.03          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 9        | 3.03          |
| (1,2482) | 1:161:A:PHE:HB2 | 1:189:A:PHE:HE2 | 17       | 3.02          |
| (1,2482) | 1:161:A:PHE:HB3 | 1:189:A:PHE:HE2 | 17       | 3.02          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 2        | 3.02          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 11       | 3.02          |
| (1,2476) | 1:161:A:PHE:HB2 | 1:189:A:PHE:HE2 | 17       | 3.02          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 3        | 3.02          |
| (1,1640) | 1:138:A:SER:HA  | 1:140:A:PHE:HD2 | 1        | 3.02          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 3        | 3.02          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 3        | 3.02          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 3        | 3.02          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 3        | 3.01          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 5        | 3.01          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 18       | 3.01          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 16       | 3.0           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 9        | 3.0           |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 10       | 3.0           |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 5        | 2.99          |
| (1,2001) | 1:161:A:PHE:HD2 | 1:162:A:ASP:H   | 17       | 2.99          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 4        | 2.99          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 12       | 2.99          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 1        | 2.99          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 1        | 2.99          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 3        | 2.98          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 20       | 2.97          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 13       | 2.97          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 13       | 2.97          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 13       | 2.97          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 6        | 2.96          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 5        | 2.96          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 5        | 2.96          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 5        | 2.96          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 6        | 2.96          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 6        | 2.96          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 6        | 2.96          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 10       | 2.95          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 7        | 2.94          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 7        | 2.94          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 8        | 2.94          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 8        | 2.94          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 8        | 2.94          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 20       | 2.94          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 8        | 2.93          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 11       | 2.93          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 11       | 2.93          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 11       | 2.93          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 14       | 2.92          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 17       | 2.92          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 18       | 2.92          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 18       | 2.92          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 18       | 2.92          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 8        | 2.9           |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 13       | 2.9           |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 13       | 2.9           |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 13       | 2.9           |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 19       | 2.89          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 20       | 2.89          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 3        | 2.89          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 20       | 2.89          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 14       | 2.88          |
| (1,1967) | 1:114:A:VAL:HB  | 1:161:A:PHE:HE2 | 15       | 2.88          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 11       | 2.88          |
| (1,2479) | 1:161:A:PHE:HD1 | 1:189:A:PHE:HZ  | 17       | 2.87          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 16       | 2.87          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 17       | 2.87          |
| (1,1641) | 1:138:A:SER:HA  | 1:140:A:PHE:HE2 | 7        | 2.86          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 16       | 2.86          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 20       | 2.86          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 20       | 2.86          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 20       | 2.86          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 11       | 2.86          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 11       | 2.86          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 11       | 2.86          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 14       | 2.86          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 14       | 2.86          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 14       | 2.86          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 19       | 2.86          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 10       | 2.86          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 10       | 2.86          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 10       | 2.86          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 19       | 2.85          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 3        | 2.85          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 3        | 2.85          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 3        | 2.85          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 12       | 2.85          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 12       | 2.85          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 12       | 2.85          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 4        | 2.85          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 16       | 2.85          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 16       | 2.85          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 16       | 2.85          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 3        | 2.84          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 3        | 2.84          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 3        | 2.84          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 15       | 2.84          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 15       | 2.84          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 15       | 2.84          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 3        | 2.84          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 7        | 2.84          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 7        | 2.84          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 7        | 2.84          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 18       | 2.83          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 17       | 2.83          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 17       | 2.83          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 17       | 2.83          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 3        | 2.82          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 11       | 2.82          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 18       | 2.82          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 19       | 2.82          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 19       | 2.82          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 19       | 2.82          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 10       | 2.82          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 10       | 2.82          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 10       | 2.82          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2  | 11       | 2.82          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2  | 11       | 2.82          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2  | 11       | 2.82          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 16       | 2.82          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 2        | 2.81          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 4        | 2.81          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 14       | 2.81          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2  | 2        | 2.81          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2  | 2        | 2.81          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2  | 2        | 2.81          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 1        | 2.81          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 13       | 2.81          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 19       | 2.81          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 6        | 2.8           |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 9        | 2.8           |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 13       | 2.8           |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 15       | 2.8           |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 17       | 2.8           |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 9        | 2.8           |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 9        | 2.8           |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 9        | 2.8           |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 18       | 2.8           |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 18       | 2.8           |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 18       | 2.8           |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2  | 14       | 2.8           |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2  | 14       | 2.8           |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2  | 14       | 2.8           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 10       | 2.8           |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 4        | 2.8           |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 1        | 2.79          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 10       | 2.79          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 12       | 2.79          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 16       | 2.79          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 19       | 2.79          |
| (1,1676) | 1:141:A:PRO:HB3 | 1:142:A:TYR:HE2 | 18       | 2.79          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2  | 6        | 2.79          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2  | 6        | 2.79          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2  | 6        | 2.79          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2  | 10       | 2.79          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2  | 10       | 2.79          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2  | 10       | 2.79          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2  | 15       | 2.79          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2  | 15       | 2.79          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2  | 15       | 2.79          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 9        | 2.79          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 5        | 2.79          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 5        | 2.79          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 5        | 2.79          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 13       | 2.78          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 13       | 2.78          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 13       | 2.78          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 2        | 2.78          |
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 2        | 2.78          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 2        | 2.78          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 18       | 2.78          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 1        | 2.78          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 1        | 2.78          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 1        | 2.78          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 7        | 2.77          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2  | 5        | 2.77          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2  | 5        | 2.77          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2  | 5        | 2.77          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 14       | 2.77          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 14       | 2.77          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 14       | 2.77          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 5        | 2.76          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 20       | 2.76          |
| (1,1676) | 1:141:A:PRO:HB3 | 1:142:A:TYR:HE2 | 7        | 2.76          |
| (1,977)  | 1:35:A:LEU:HD21 | 1:86:A:PHE:HE1  | 7        | 2.76          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,977)  | 1:35:A:LEU:HD22 | 1:86:A:PHE:HE1  | 7        | 2.76          |
| (1,977)  | 1:35:A:LEU:HD23 | 1:86:A:PHE:HE1  | 7        | 2.76          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2  | 7        | 2.76          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2  | 7        | 2.76          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2  | 7        | 2.76          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 1        | 2.76          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 13       | 2.76          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 6        | 2.76          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 6        | 2.76          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 6        | 2.76          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 2        | 2.75          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 7        | 2.75          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 10       | 2.75          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 19       | 2.75          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 19       | 2.75          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 19       | 2.75          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 4        | 2.74          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 9        | 2.74          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 2        | 2.74          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 2        | 2.74          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 2        | 2.74          |
| (1,2477) | 1:161:A:PHE:HE1 | 1:189:A:PHE:HE2 | 8        | 2.73          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 2        | 2.73          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 2        | 2.73          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 2        | 2.73          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 17       | 2.73          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 17       | 2.73          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 17       | 2.73          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 2        | 2.73          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 2        | 2.73          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 2        | 2.73          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 4        | 2.72          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 5        | 2.72          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 6        | 2.72          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 8        | 2.72          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 12       | 2.72          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 3        | 2.72          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 10       | 2.72          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 8        | 2.72          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 11       | 2.72          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 12       | 2.72          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 16       | 2.71          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 16       | 2.71          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 16       | 2.71          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 18       | 2.7           |
| (1,1055) | 1:94:A:SER:HA   | 1:95:A:PHE:HE2  | 5        | 2.7           |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 2        | 2.7           |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 7        | 2.7           |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 2        | 2.69          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 12       | 2.69          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2  | 3        | 2.69          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2  | 3        | 2.69          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2  | 3        | 2.69          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 15       | 2.69          |
| (1,2495) | 1:182:A:LYS:HB2 | 1:189:A:PHE:HE2 | 17       | 2.68          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 17       | 2.68          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 5        | 2.68          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 4        | 2.68          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 4        | 2.68          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 4        | 2.68          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 3        | 2.68          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 8        | 2.67          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3 | 8        | 2.67          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 7        | 2.67          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 7        | 2.67          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 7        | 2.67          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 10       | 2.67          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 10       | 2.67          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 10       | 2.67          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 11       | 2.67          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 11       | 2.67          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 11       | 2.67          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 6        | 2.67          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 8        | 2.67          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 11       | 2.67          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 12       | 2.67          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 10       | 2.67          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 19       | 2.66          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3 | 19       | 2.66          |
| (1,1676) | 1:141:A:PRO:HB3 | 1:142:A:TYR:HE2 | 1        | 2.66          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 20       | 2.65          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3 | 20       | 2.65          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 18       | 2.65          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 18       | 2.65          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 18       | 2.65          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 15       | 2.65          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 15       | 2.65          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 15       | 2.65          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 5        | 2.64          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 5        | 2.64          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 5        | 2.64          |
| (1,119)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 14       | 2.64          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 15       | 2.64          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 11       | 2.64          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 13       | 2.64          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 19       | 2.63          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 19       | 2.63          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 19       | 2.63          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 5        | 2.63          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 7        | 2.63          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 18       | 2.63          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2  | 9        | 2.62          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2  | 9        | 2.62          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2  | 9        | 2.62          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 6        | 2.62          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 1        | 2.62          |
| (1,2512) | 1:188:A:GLY:HA2 | 1:189:A:PHE:HD1 | 17       | 2.61          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 7        | 2.61          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3 | 7        | 2.61          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 12       | 2.61          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3 | 12       | 2.61          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 14       | 2.61          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 14       | 2.61          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 14       | 2.61          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2 | 7        | 2.61          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2  | 13       | 2.61          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2  | 13       | 2.61          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2  | 13       | 2.61          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 4        | 2.61          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 5        | 2.6           |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 16       | 2.6           |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 16       | 2.6           |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 17       | 2.6           |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 11       | 2.59          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3 | 11       | 2.59          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 20       | 2.59          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 20       | 2.59          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 20       | 2.59          |
| (1,115)  | 1:21:A:ARG:HB3  | 1:22:A:PHE:HE2  | 14       | 2.59          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 15       | 2.59          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 16       | 2.59          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 17       | 2.58          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3 | 17       | 2.58          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 10       | 2.58          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 10       | 2.58          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 10       | 2.58          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 2        | 2.58          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 5        | 2.58          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 6        | 2.58          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 14       | 2.58          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 5        | 2.57          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3 | 5        | 2.57          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 10       | 2.57          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3 | 10       | 2.57          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 8        | 2.57          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 8        | 2.57          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 8        | 2.57          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 1        | 2.57          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2  | 20       | 2.57          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 6        | 2.56          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 6        | 2.56          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 6        | 2.56          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 7        | 2.56          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 7        | 2.56          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 7        | 2.56          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2 | 11       | 2.56          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2 | 11       | 2.56          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2 | 11       | 2.56          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1  | 5        | 2.56          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1  | 5        | 2.56          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1  | 5        | 2.56          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 8        | 2.56          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 8        | 2.56          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 3        | 2.55          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3 | 3        | 2.55          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 9        | 2.55          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3 | 9        | 2.55          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2 | 16       | 2.55          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3  | 16       | 2.55          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2  | 15       | 2.54          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3  | 15       | 2.54          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 11       | 2.54          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 11       | 2.54          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 11       | 2.54          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2  | 3        | 2.54          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2  | 3        | 2.54          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2  | 3        | 2.54          |
| (1,1678) | 1:141:A:PRO:HA  | 1:142:A:TYR:HD2  | 20       | 2.54          |
| (1,1641) | 1:138:A:SER:HA  | 1:140:A:PHE:HE2  | 9        | 2.54          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2   | 16       | 2.54          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2   | 16       | 2.54          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2   | 16       | 2.54          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1   | 19       | 2.54          |
| (1,2463) | 1:123:A:ASP:HB2 | 1:189:A:PHE:HE1  | 17       | 2.53          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2  | 1        | 2.53          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3  | 1        | 2.53          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 3        | 2.53          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 3        | 2.53          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 3        | 2.53          |
| (1,1678) | 1:141:A:PRO:HA  | 1:142:A:TYR:HD2  | 16       | 2.53          |
| (1,1676) | 1:141:A:PRO:HB3 | 1:142:A:TYR:HE2  | 11       | 2.53          |
| (1,2496) | 1:182:A:LYS:HG3 | 1:189:A:PHE:HE2  | 17       | 2.52          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2  | 2        | 2.52          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3  | 2        | 2.52          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2  | 18       | 2.52          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3  | 18       | 2.52          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 18       | 2.52          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 18       | 2.52          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 18       | 2.52          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 18       | 2.52          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2  | 9        | 2.52          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1   | 6        | 2.52          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2   | 4        | 2.52          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2   | 4        | 2.52          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2   | 4        | 2.52          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2   | 12       | 2.52          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2   | 12       | 2.52          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2   | 12       | 2.52          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2   | 16       | 2.52          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2   | 17       | 2.52          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 2        | 2.51          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 2        | 2.51          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 2        | 2.51          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 4        | 2.51          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 4        | 2.51          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 4        | 2.51          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 19       | 2.51          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 19       | 2.51          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 19       | 2.51          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2  | 15       | 2.51          |
| (1,1645) | 1:139:A:LEU:HA  | 1:140:A:PHE:HD2  | 1        | 2.51          |
| (1,1641) | 1:138:A:SER:HA  | 1:140:A:PHE:HE2  | 1        | 2.51          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1   | 8        | 2.51          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1   | 13       | 2.51          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1   | 6        | 2.51          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1   | 6        | 2.51          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1   | 6        | 2.51          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2  | 9        | 2.5           |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2  | 9        | 2.5           |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2  | 9        | 2.5           |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2  | 13       | 2.5           |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2  | 13       | 2.5           |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2  | 13       | 2.5           |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2  | 15       | 2.5           |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2  | 15       | 2.5           |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2  | 15       | 2.5           |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2   | 17       | 2.5           |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2   | 17       | 2.5           |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2   | 17       | 2.5           |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2  | 6        | 2.49          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3  | 6        | 2.49          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2  | 13       | 2.49          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3  | 13       | 2.49          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2  | 14       | 2.49          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3  | 14       | 2.49          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 7        | 2.49          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 7        | 2.49          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 7        | 2.49          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 10       | 2.49          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 10       | 2.49          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 10       | 2.49          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 13       | 2.49          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 13       | 2.49          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 13       | 2.49          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 15       | 2.49          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 15       | 2.49          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 15       | 2.49          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 2        | 2.49          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 14       | 2.49          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2  | 1        | 2.49          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2  | 1        | 2.49          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2  | 1        | 2.49          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2  | 12       | 2.49          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2  | 12       | 2.49          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2  | 12       | 2.49          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2   | 1        | 2.49          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2   | 1        | 2.49          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2   | 1        | 2.49          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2   | 19       | 2.49          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2   | 19       | 2.49          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2   | 19       | 2.49          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2   | 20       | 2.49          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3   | 20       | 2.49          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1   | 20       | 2.49          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1   | 20       | 2.49          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1   | 20       | 2.49          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1   | 3        | 2.49          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1   | 3        | 2.49          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1   | 3        | 2.49          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB2  | 4        | 2.48          |
| (1,2409) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HB3  | 4        | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 1        | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 1        | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 1        | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 6        | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 6        | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 6        | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 9        | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 9        | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 9        | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 12       | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 12       | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 12       | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 14       | 2.48          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 14       | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 14       | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 16       | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 16       | 2.48          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 16       | 2.48          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2  | 18       | 2.48          |
| (1,1970) | 1:150:A:ALA:HB1 | 1:161:A:PHE:HE2  | 4        | 2.48          |
| (1,1970) | 1:150:A:ALA:HB2 | 1:161:A:PHE:HE2  | 4        | 2.48          |
| (1,1970) | 1:150:A:ALA:HB3 | 1:161:A:PHE:HE2  | 4        | 2.48          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2  | 11       | 2.48          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1   | 15       | 2.48          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1   | 15       | 2.48          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1   | 15       | 2.48          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2   | 8        | 2.48          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2   | 8        | 2.48          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2   | 8        | 2.48          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2   | 17       | 2.48          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3   | 17       | 2.48          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1   | 8        | 2.48          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1   | 8        | 2.48          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1   | 8        | 2.48          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 4        | 2.47          |
| (1,1678) | 1:141:A:PRO:HA  | 1:142:A:TYR:HD2  | 7        | 2.47          |
| (1,982)  | 1:59:A:VAL:HG21 | 1:86:A:PHE:HD1   | 14       | 2.47          |
| (1,982)  | 1:59:A:VAL:HG22 | 1:86:A:PHE:HD1   | 14       | 2.47          |
| (1,982)  | 1:59:A:VAL:HG23 | 1:86:A:PHE:HD1   | 14       | 2.47          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1   | 8        | 2.47          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 5        | 2.46          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 5        | 2.46          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 5        | 2.46          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 17       | 2.46          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 17       | 2.46          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 17       | 2.46          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2  | 2        | 2.46          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 3        | 2.46          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 6        | 2.46          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 16       | 2.46          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2   | 18       | 2.46          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2   | 18       | 2.46          |
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2   | 18       | 2.46          |
| (1,962)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HE2   | 20       | 2.46          |
| (1,962)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HE2   | 20       | 2.46          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,962)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HE2   | 20       | 2.46          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 20       | 2.45          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 20       | 2.45          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 20       | 2.45          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2  | 6        | 2.45          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 11       | 2.45          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG21 | 8        | 2.44          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG22 | 8        | 2.44          |
| (1,2361) | 1:161:A:PHE:HD1 | 1:180:A:VAL:HG23 | 8        | 2.44          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 10       | 2.44          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 13       | 2.44          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2  | 19       | 2.44          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2   | 3        | 2.44          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2  | 14       | 2.43          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2  | 4        | 2.42          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2  | 16       | 2.42          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 1        | 2.42          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 15       | 2.42          |
| (1,1055) | 1:94:A:SER:HA   | 1:95:A:PHE:HE2   | 19       | 2.42          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2   | 8        | 2.42          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2   | 12       | 2.42          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1   | 11       | 2.42          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1   | 11       | 2.42          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1   | 11       | 2.42          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1   | 13       | 2.42          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1   | 13       | 2.42          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1   | 13       | 2.42          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2  | 3        | 2.41          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2  | 11       | 2.41          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2  | 13       | 2.41          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 7        | 2.41          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 19       | 2.41          |
| (1,1678) | 1:141:A:PRO:HA  | 1:142:A:TYR:HD2  | 1        | 2.41          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2  | 9        | 2.41          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2  | 14       | 2.41          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1   | 7        | 2.41          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1   | 7        | 2.41          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1   | 7        | 2.41          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1   | 18       | 2.41          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1   | 18       | 2.41          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1   | 18       | 2.41          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2  | 9        | 2.4           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 17       | 2.4           |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2  | 9        | 2.4           |
| (1,1678) | 1:141:A:PRO:HA  | 1:142:A:TYR:HD2 | 18       | 2.39          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 11       | 2.39          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 9        | 2.39          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 9        | 2.39          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 9        | 2.39          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2 | 1        | 2.38          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2 | 10       | 2.38          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2 | 15       | 2.38          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2 | 19       | 2.38          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2 | 5        | 2.38          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2 | 12       | 2.38          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 15       | 2.38          |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 20       | 2.38          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 20       | 2.38          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 20       | 2.38          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 9        | 2.38          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1  | 17       | 2.38          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1  | 17       | 2.38          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1  | 17       | 2.38          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2 | 20       | 2.37          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 6        | 2.37          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 12       | 2.37          |
| (1,111)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HE1  | 12       | 2.37          |
| (1,111)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HE1  | 12       | 2.37          |
| (1,111)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HE1  | 12       | 2.37          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1  | 10       | 2.37          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1  | 10       | 2.37          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1  | 10       | 2.37          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2 | 9        | 2.36          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2 | 17       | 2.36          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 4        | 2.36          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 5        | 2.36          |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 8        | 2.36          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 8        | 2.36          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 8        | 2.36          |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 18       | 2.36          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 18       | 2.36          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 18       | 2.36          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 9        | 2.36          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 9        | 2.36          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1  | 19       | 2.36          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1  | 19       | 2.36          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1  | 19       | 2.36          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2 | 7        | 2.35          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 8        | 2.35          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 13       | 2.35          |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 19       | 2.35          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 19       | 2.35          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 19       | 2.35          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2  | 4        | 2.35          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1  | 1        | 2.35          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1  | 1        | 2.35          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1  | 1        | 2.35          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1  | 16       | 2.35          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1  | 16       | 2.35          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1  | 16       | 2.35          |
| (1,2464) | 1:123:A:ASP:HB2 | 1:189:A:PHE:HE1 | 17       | 2.34          |
| (1,2464) | 1:123:A:ASP:HB3 | 1:189:A:PHE:HE1 | 17       | 2.34          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2 | 5        | 2.34          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 20       | 2.34          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2 | 12       | 2.33          |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 9        | 2.33          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 9        | 2.33          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 9        | 2.33          |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 12       | 2.33          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 12       | 2.33          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 12       | 2.33          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2  | 18       | 2.33          |
| (1,108)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 12       | 2.33          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2 | 17       | 2.32          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2 | 20       | 2.32          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 10       | 2.32          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 12       | 2.32          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 12       | 2.32          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2  | 2        | 2.32          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 10       | 2.32          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 10       | 2.32          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2  | 19       | 2.31          |
| (1,2540) | 1:189:A:PHE:HD2 | 1:190:A:ASN:H   | 17       | 2.3           |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 13       | 2.3           |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 13       | 2.3           |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 13       | 2.3           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,118)  | 1:21:A:ARG:HG3   | 1:22:A:PHE:HD2  | 1        | 2.3           |
| (1,105)  | 1:19:A:LEU:HD11  | 1:22:A:PHE:HD1  | 4        | 2.3           |
| (1,105)  | 1:19:A:LEU:HD12  | 1:22:A:PHE:HD1  | 4        | 2.3           |
| (1,105)  | 1:19:A:LEU:HD13  | 1:22:A:PHE:HD1  | 4        | 2.3           |
| (1,2494) | 1:182:A:LYS:HA   | 1:189:A:PHE:HD2 | 17       | 2.29          |
| (1,2462) | 1:123:A:ASP:HB3  | 1:189:A:PHE:HE1 | 17       | 2.29          |
| (1,1678) | 1:141:A:PRO:HA   | 1:142:A:TYR:HD2 | 11       | 2.29          |
| (1,980)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HD1  | 10       | 2.29          |
| (1,980)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HD1  | 10       | 2.29          |
| (1,980)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HD1  | 10       | 2.29          |
| (1,980)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HD1  | 14       | 2.29          |
| (1,980)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HD1  | 14       | 2.29          |
| (1,980)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HD1  | 14       | 2.29          |
| (1,980)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HD1  | 15       | 2.29          |
| (1,980)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HD1  | 15       | 2.29          |
| (1,980)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HD1  | 15       | 2.29          |
| (1,1646) | 1:139:A:LEU:HB2  | 1:140:A:PHE:HD2 | 10       | 2.28          |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2 | 20       | 2.28          |
| (1,985)  | 1:68:A:TYR:HB2   | 1:86:A:PHE:HD1  | 3        | 2.28          |
| (1,118)  | 1:21:A:ARG:HG3   | 1:22:A:PHE:HD2  | 13       | 2.28          |
| (1,107)  | 1:19:A:LEU:HB2   | 1:22:A:PHE:HE1  | 7        | 2.28          |
| (1,107)  | 1:19:A:LEU:HB3   | 1:22:A:PHE:HE1  | 7        | 2.28          |
| (1,2504) | 1:182:A:LYS:HB2  | 1:189:A:PHE:HE2 | 17       | 2.27          |
| (1,2504) | 1:182:A:LYS:HB3  | 1:189:A:PHE:HE2 | 17       | 2.27          |
| (1,2490) | 1:180:A:VAL:HG11 | 1:189:A:PHE:HE2 | 17       | 2.27          |
| (1,2490) | 1:180:A:VAL:HG12 | 1:189:A:PHE:HE2 | 17       | 2.27          |
| (1,2490) | 1:180:A:VAL:HG13 | 1:189:A:PHE:HE2 | 17       | 2.27          |
| (1,2480) | 1:161:A:PHE:HZ   | 1:189:A:PHE:HE2 | 17       | 2.27          |
| (1,980)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HD1  | 5        | 2.27          |
| (1,980)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HD1  | 5        | 2.27          |
| (1,980)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HD1  | 5        | 2.27          |
| (1,980)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HD1  | 11       | 2.27          |
| (1,980)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HD1  | 11       | 2.27          |
| (1,980)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HD1  | 11       | 2.27          |
| (1,107)  | 1:19:A:LEU:HB2   | 1:22:A:PHE:HE1  | 1        | 2.27          |
| (1,107)  | 1:19:A:LEU:HB3   | 1:22:A:PHE:HE1  | 1        | 2.27          |
| (1,107)  | 1:19:A:LEU:HB2   | 1:22:A:PHE:HE1  | 15       | 2.27          |
| (1,107)  | 1:19:A:LEU:HB3   | 1:22:A:PHE:HE1  | 15       | 2.27          |
| (1,1646) | 1:139:A:LEU:HB2  | 1:140:A:PHE:HD2 | 13       | 2.26          |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2 | 16       | 2.26          |
| (1,980)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HD1  | 6        | 2.26          |
| (1,980)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HD1  | 6        | 2.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 6        | 2.26          |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 7        | 2.26          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 7        | 2.26          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 7        | 2.26          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2  | 7        | 2.26          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 3        | 2.26          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 3        | 2.26          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 5        | 2.26          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 5        | 2.26          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 6        | 2.26          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 6        | 2.26          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 11       | 2.26          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 11       | 2.26          |
| (1,1640) | 1:138:A:SER:HA  | 1:140:A:PHE:HD2 | 20       | 2.25          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 9        | 2.25          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 11       | 2.25          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 4        | 2.25          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 4        | 2.25          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 13       | 2.25          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 13       | 2.25          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 14       | 2.25          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 14       | 2.25          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1  | 2        | 2.25          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1  | 2        | 2.25          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1  | 2        | 2.25          |
| (1,1974) | 1:152:A:ALA:HA  | 1:161:A:PHE:HD2 | 8        | 2.24          |
| (1,1055) | 1:94:A:SER:HA   | 1:95:A:PHE:HE2  | 4        | 2.24          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 7        | 2.24          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 2        | 2.24          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 2        | 2.24          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 17       | 2.24          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 17       | 2.24          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 18       | 2.24          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 18       | 2.24          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1  | 5        | 2.24          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1  | 5        | 2.24          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1  | 5        | 2.24          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1  | 20       | 2.24          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1  | 20       | 2.24          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1  | 20       | 2.24          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 18       | 2.23          |
| (1,1640) | 1:138:A:SER:HA  | 1:140:A:PHE:HD2 | 16       | 2.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 3        | 2.23          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 3        | 2.23          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 3        | 2.23          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE2  | 7        | 2.23          |
| (1,870)  | 1:22:A:PHE:HE1  | 1:81:A:LYS:HE3  | 7        | 2.23          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 16       | 2.23          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 16       | 2.23          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1  | 6        | 2.23          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1  | 6        | 2.23          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1  | 6        | 2.23          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 7        | 2.22          |
| (1,1055) | 1:94:A:SER:HA   | 1:95:A:PHE:HE2  | 15       | 2.22          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2  | 11       | 2.22          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 11       | 2.21          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 11       | 2.21          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 11       | 2.21          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2  | 14       | 2.21          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1  | 14       | 2.21          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1  | 14       | 2.21          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1  | 14       | 2.21          |
| (1,2499) | 1:182:A:LYS:HA  | 1:189:A:PHE:HE2 | 17       | 2.2           |
| (1,2498) | 1:182:A:LYS:HB3 | 1:189:A:PHE:HE2 | 17       | 2.2           |
| (1,1055) | 1:94:A:SER:HA   | 1:95:A:PHE:HE2  | 8        | 2.2           |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 4        | 2.2           |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 4        | 2.2           |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 4        | 2.2           |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 14       | 2.2           |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 14       | 2.2           |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 14       | 2.2           |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 19       | 2.2           |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 19       | 2.2           |
| (1,1055) | 1:94:A:SER:HA   | 1:95:A:PHE:HE2  | 2        | 2.19          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 2        | 2.19          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 2        | 2.19          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 2        | 2.19          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 8        | 2.19          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 8        | 2.19          |
| (1,1975) | 1:152:A:ALA:HA  | 1:161:A:PHE:HE2 | 8        | 2.18          |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 2        | 2.18          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 2        | 2.18          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 2        | 2.18          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 10       | 2.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 10       | 2.18          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 10       | 2.18          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 15       | 2.18          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 15       | 2.18          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 15       | 2.18          |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 1        | 2.17          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 1        | 2.17          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 1        | 2.17          |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 16       | 2.17          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 16       | 2.17          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 16       | 2.17          |
| (1,2505) | 1:182:A:LYS:HG2 | 1:189:A:PHE:HE2 | 17       | 2.16          |
| (1,2505) | 1:182:A:LYS:HG3 | 1:189:A:PHE:HE2 | 17       | 2.16          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 2        | 2.16          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 6        | 2.16          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 6        | 2.16          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 6        | 2.16          |
| (1,980)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HD1  | 17       | 2.15          |
| (1,980)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HD1  | 17       | 2.15          |
| (1,980)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HD1  | 17       | 2.15          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 15       | 2.14          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 9        | 2.14          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 9        | 2.14          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 12       | 2.13          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 12       | 2.13          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 1        | 2.12          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 16       | 2.12          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 5        | 2.12          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 5        | 2.12          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 5        | 2.12          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 7        | 2.11          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 7        | 2.11          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 7        | 2.11          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1  | 15       | 2.11          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1  | 15       | 2.11          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1  | 15       | 2.11          |
| (1,1646) | 1:139:A:LEU:HB2 | 1:140:A:PHE:HD2 | 3        | 2.1           |
| (1,1055) | 1:94:A:SER:HA   | 1:95:A:PHE:HE2  | 9        | 2.1           |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2  | 2        | 2.09          |
| (1,107)  | 1:19:A:LEU:HB2  | 1:22:A:PHE:HE1  | 20       | 2.09          |
| (1,107)  | 1:19:A:LEU:HB3  | 1:22:A:PHE:HE1  | 20       | 2.09          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2 | 14       | 2.08          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1   | 14       | 2.08          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 7        | 2.08          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2  | 2        | 2.06          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1   | 17       | 2.06          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 11       | 2.06          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2   | 3        | 2.06          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2   | 3        | 2.06          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2   | 3        | 2.06          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1   | 9        | 2.06          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1   | 9        | 2.06          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1   | 9        | 2.06          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 5        | 2.05          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 6        | 2.05          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1   | 8        | 2.04          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1   | 8        | 2.04          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1   | 8        | 2.04          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 10       | 2.03          |
| (1,105)  | 1:19:A:LEU:HD11 | 1:22:A:PHE:HD1   | 12       | 2.03          |
| (1,105)  | 1:19:A:LEU:HD12 | 1:22:A:PHE:HD1   | 12       | 2.03          |
| (1,105)  | 1:19:A:LEU:HD13 | 1:22:A:PHE:HD1   | 12       | 2.03          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 15       | 2.02          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2   | 15       | 2.02          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1   | 3        | 2.01          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 14       | 2.0           |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2   | 9        | 2.0           |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2   | 9        | 2.0           |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2   | 9        | 2.0           |
| (1,2542) | 1:189:A:PHE:HD2 | 1:190:A:ASN:HD22 | 17       | 1.99          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1   | 14       | 1.99          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1   | 14       | 1.99          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1   | 14       | 1.99          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1   | 20       | 1.98          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2   | 5        | 1.98          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2   | 6        | 1.98          |
| (1,118)  | 1:21:A:ARG:HG3  | 1:22:A:PHE:HD2   | 10       | 1.98          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1   | 18       | 1.97          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1   | 15       | 1.97          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1   | 15       | 1.97          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1   | 15       | 1.97          |
| (1,2515) | 1:189:A:PHE:H   | 1:189:A:PHE:HD1  | 17       | 1.96          |
| (1,2514) | 1:188:A:GLY:HA2 | 1:189:A:PHE:HE1  | 17       | 1.96          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 3        | 1.96          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 13       | 1.96          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 13       | 1.96          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 13       | 1.96          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1  | 11       | 1.96          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1  | 13       | 1.96          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1  | 18       | 1.96          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2 | 17       | 1.95          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3 | 17       | 1.95          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 1        | 1.95          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 1        | 1.95          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 1        | 1.95          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 16       | 1.95          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 16       | 1.95          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 16       | 1.95          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1  | 6        | 1.95          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1  | 6        | 1.95          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1  | 6        | 1.95          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2 | 9        | 1.94          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3 | 9        | 1.94          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1  | 10       | 1.94          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1  | 5        | 1.94          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1  | 5        | 1.94          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1  | 5        | 1.94          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2 | 7        | 1.93          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3 | 7        | 1.93          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2 | 20       | 1.93          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3 | 20       | 1.93          |
| (1,1689) | 1:142:A:TYR:HD1 | 1:143:A:GLU:H   | 7        | 1.93          |
| (1,985)  | 1:68:A:TYR:HB2  | 1:86:A:PHE:HD1  | 19       | 1.93          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 19       | 1.93          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 19       | 1.93          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 19       | 1.93          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1  | 4        | 1.93          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1  | 2        | 1.93          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1  | 2        | 1.93          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1  | 2        | 1.93          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1  | 10       | 1.93          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1  | 10       | 1.93          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1  | 10       | 1.93          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1  | 11       | 1.93          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1  | 11       | 1.93          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1  | 11       | 1.93          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1  | 13       | 1.93          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1  | 13       | 1.93          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1  | 13       | 1.93          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1  | 18       | 1.93          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1  | 18       | 1.93          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1  | 18       | 1.93          |
| (1,1651) | 1:140:A:PHE:H   | 1:140:A:PHE:HD2 | 4        | 1.92          |
| (1,1651) | 1:140:A:PHE:H   | 1:140:A:PHE:HD2 | 5        | 1.92          |
| (1,1651) | 1:140:A:PHE:H   | 1:140:A:PHE:HD2 | 6        | 1.92          |
| (1,1651) | 1:140:A:PHE:H   | 1:140:A:PHE:HD2 | 8        | 1.92          |
| (1,1651) | 1:140:A:PHE:H   | 1:140:A:PHE:HD2 | 12       | 1.92          |
| (1,1055) | 1:94:A:SER:HA   | 1:95:A:PHE:HE2  | 12       | 1.92          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 12       | 1.92          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 12       | 1.92          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 12       | 1.92          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 18       | 1.92          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 18       | 1.92          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 18       | 1.92          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1  | 1        | 1.92          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1  | 3        | 1.92          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1  | 3        | 1.92          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1  | 3        | 1.92          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1  | 8        | 1.92          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1  | 8        | 1.92          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1  | 8        | 1.92          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2 | 4        | 1.91          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3 | 4        | 1.91          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2 | 13       | 1.91          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3 | 13       | 1.91          |
| (1,1640) | 1:138:A:SER:HA  | 1:140:A:PHE:HD2 | 13       | 1.91          |
| (1,988)  | 1:85:A:GLU:HA   | 1:86:A:PHE:HE2  | 16       | 1.91          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 4        | 1.91          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 4        | 1.91          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 4        | 1.91          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2  | 20       | 1.91          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2  | 20       | 1.91          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2  | 20       | 1.91          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1  | 7        | 1.91          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1  | 16       | 1.91          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1  | 16       | 1.91          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1  | 16       | 1.91          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2 | 15       | 1.9           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 15       | 1.9           |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG11 | 20       | 1.9           |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG12 | 20       | 1.9           |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG13 | 20       | 1.9           |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2  | 2        | 1.9           |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1   | 2        | 1.9           |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1   | 14       | 1.9           |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1   | 1        | 1.9           |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1   | 1        | 1.9           |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1   | 1        | 1.9           |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1   | 7        | 1.9           |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1   | 7        | 1.9           |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1   | 7        | 1.9           |
| (1,2513) | 1:188:A:GLY:HA3 | 1:189:A:PHE:HD1  | 17       | 1.89          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 8        | 1.89          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 8        | 1.89          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 19       | 1.89          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 19       | 1.89          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG11 | 18       | 1.89          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG12 | 18       | 1.89          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG13 | 18       | 1.89          |
| (1,1689) | 1:142:A:TYR:HD1 | 1:143:A:GLU:H    | 20       | 1.89          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2   | 8        | 1.89          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2   | 8        | 1.89          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2   | 8        | 1.89          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1   | 15       | 1.89          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1   | 16       | 1.89          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 1        | 1.88          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 1        | 1.88          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 10       | 1.88          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 10       | 1.88          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 12       | 1.88          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 12       | 1.88          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG11 | 1        | 1.88          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG12 | 1        | 1.88          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG13 | 1        | 1.88          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG21 | 1        | 1.88          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG22 | 1        | 1.88          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG23 | 1        | 1.88          |
| (1,963)  | 1:23:A:ALA:HB1  | 1:86:A:PHE:HD2   | 17       | 1.88          |
| (1,963)  | 1:23:A:ALA:HB2  | 1:86:A:PHE:HD2   | 17       | 1.88          |
| (1,963)  | 1:23:A:ALA:HB3  | 1:86:A:PHE:HD2   | 17       | 1.88          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1   | 17       | 1.88          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 3        | 1.87          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 3        | 1.87          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 5        | 1.87          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 5        | 1.87          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 14       | 1.87          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 14       | 1.87          |
| (1,1689) | 1:142:A:TYR:HD1 | 1:143:A:GLU:H    | 1        | 1.87          |
| (1,1640) | 1:138:A:SER:HA  | 1:140:A:PHE:HD2  | 2        | 1.87          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 9        | 1.87          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 6        | 1.86          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 6        | 1.86          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 11       | 1.86          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 11       | 1.86          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 18       | 1.86          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 18       | 1.86          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG11 | 7        | 1.86          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG12 | 7        | 1.86          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG13 | 7        | 1.86          |
| (1,1689) | 1:142:A:TYR:HD1 | 1:143:A:GLU:H    | 11       | 1.86          |
| (1,1689) | 1:142:A:TYR:HD1 | 1:143:A:GLU:H    | 18       | 1.86          |
| (1,1651) | 1:140:A:PHE:H   | 1:140:A:PHE:HD2  | 7        | 1.86          |
| (1,1638) | 1:138:A:SER:HB2 | 1:140:A:PHE:HE2  | 20       | 1.86          |
| (1,988)  | 1:85:A:GLU:HA   | 1:86:A:PHE:HE2   | 3        | 1.86          |
| (1,988)  | 1:85:A:GLU:HA   | 1:86:A:PHE:HE2   | 17       | 1.86          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1   | 6        | 1.86          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1   | 17       | 1.86          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1   | 17       | 1.86          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1   | 17       | 1.86          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1   | 5        | 1.85          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1   | 4        | 1.85          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1   | 4        | 1.85          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1   | 4        | 1.85          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1   | 19       | 1.85          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1   | 19       | 1.85          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1   | 19       | 1.85          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG2  | 17       | 1.84          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG3  | 17       | 1.84          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG2  | 20       | 1.84          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG3  | 20       | 1.84          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG2  | 16       | 1.84          |
| (1,2410) | 1:161:A:PHE:HD1 | 1:182:A:LYS:HG3  | 16       | 1.84          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2 | 9        | 1.84          |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2  | 8        | 1.84          |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2  | 13       | 1.84          |
| (1,970)  | 1:25:A:ASP:H     | 1:86:A:PHE:HE2  | 13       | 1.84          |
| (1,2410) | 1:161:A:PHE:HD1  | 1:182:A:LYS:HG2 | 2        | 1.83          |
| (1,2410) | 1:161:A:PHE:HD1  | 1:182:A:LYS:HG3 | 2        | 1.83          |
| (1,1689) | 1:142:A:TYR:HD1  | 1:143:A:GLU:H   | 16       | 1.83          |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2  | 19       | 1.83          |
| (1,112)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HE1  | 19       | 1.83          |
| (1,109)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HE1  | 12       | 1.83          |
| (1,109)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HE1  | 12       | 1.83          |
| (1,109)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HE1  | 12       | 1.83          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2 | 8        | 1.82          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3 | 8        | 1.82          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2 | 9        | 1.82          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3 | 9        | 1.82          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2 | 1        | 1.82          |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2  | 9        | 1.82          |
| (1,109)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HE1  | 9        | 1.82          |
| (1,109)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HE1  | 9        | 1.82          |
| (1,109)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HE1  | 9        | 1.82          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 8        | 1.82          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 8        | 1.82          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 8        | 1.82          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2 | 7        | 1.81          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3 | 7        | 1.81          |
| (1,1668) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HD1 | 11       | 1.81          |
| (1,1668) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HD1 | 11       | 1.81          |
| (1,1668) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HD1 | 11       | 1.81          |
| (1,1640) | 1:138:A:SER:HA   | 1:140:A:PHE:HD2 | 14       | 1.8           |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2  | 2        | 1.8           |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2  | 4        | 1.8           |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 9        | 1.8           |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 9        | 1.8           |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 9        | 1.8           |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 12       | 1.8           |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 12       | 1.8           |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 12       | 1.8           |
| (1,2489) | 1:180:A:VAL:HG21 | 1:189:A:PHE:HE2 | 17       | 1.79          |
| (1,2489) | 1:180:A:VAL:HG22 | 1:189:A:PHE:HE2 | 17       | 1.79          |
| (1,2489) | 1:180:A:VAL:HG23 | 1:189:A:PHE:HE2 | 17       | 1.79          |
| (1,1640) | 1:138:A:SER:HA   | 1:140:A:PHE:HD2 | 17       | 1.79          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2   | 5        | 1.79          |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2   | 15       | 1.79          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1   | 12       | 1.79          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1   | 12       | 1.79          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1   | 12       | 1.79          |
| (1,116)  | 1:21:A:ARG:HG2   | 1:22:A:PHE:HE2   | 3        | 1.79          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1   | 2        | 1.79          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1   | 2        | 1.79          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1   | 2        | 1.79          |
| (1,2486) | 1:180:A:VAL:HG11 | 1:189:A:PHE:HD2  | 17       | 1.78          |
| (1,2486) | 1:180:A:VAL:HG12 | 1:189:A:PHE:HD2  | 17       | 1.78          |
| (1,2486) | 1:180:A:VAL:HG13 | 1:189:A:PHE:HD2  | 17       | 1.78          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2  | 5        | 1.78          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3  | 5        | 1.78          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2  | 12       | 1.78          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3  | 12       | 1.78          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2  | 13       | 1.78          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3  | 13       | 1.78          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2  | 15       | 1.78          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3  | 15       | 1.78          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2  | 19       | 1.78          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3  | 19       | 1.78          |
| (1,1640) | 1:138:A:SER:HA   | 1:140:A:PHE:HD2  | 11       | 1.78          |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2   | 11       | 1.78          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2  | 1        | 1.77          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3  | 1        | 1.77          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2  | 4        | 1.77          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3  | 4        | 1.77          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2  | 10       | 1.77          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3  | 10       | 1.77          |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2   | 7        | 1.77          |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2   | 10       | 1.77          |
| (1,970)  | 1:25:A:ASP:H     | 1:86:A:PHE:HE2   | 4        | 1.77          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1   | 1        | 1.77          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1   | 1        | 1.77          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1   | 1        | 1.77          |
| (1,2101) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG11 | 1        | 1.76          |
| (1,2101) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG12 | 1        | 1.76          |
| (1,2101) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG13 | 1        | 1.76          |
| (1,1668) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HD1  | 7        | 1.76          |
| (1,1668) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HD1  | 7        | 1.76          |
| (1,1668) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HD1  | 7        | 1.76          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1668) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HD1 | 16       | 1.76          |
| (1,1668) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HD1 | 16       | 1.76          |
| (1,1668) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HD1 | 16       | 1.76          |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2  | 14       | 1.76          |
| (1,116)  | 1:21:A:ARG:HG2   | 1:22:A:PHE:HE2  | 18       | 1.76          |
| (1,112)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HE1  | 8        | 1.76          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 4        | 1.76          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 4        | 1.76          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 4        | 1.76          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 6        | 1.76          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 6        | 1.76          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 6        | 1.76          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 7        | 1.76          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 7        | 1.76          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 7        | 1.76          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 19       | 1.76          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 19       | 1.76          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 19       | 1.76          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2 | 6        | 1.75          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3 | 6        | 1.75          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2 | 14       | 1.75          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3 | 14       | 1.75          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG2 | 16       | 1.75          |
| (1,2411) | 1:161:A:PHE:HE1  | 1:182:A:LYS:HG3 | 16       | 1.75          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 10       | 1.75          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 10       | 1.75          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 10       | 1.75          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 13       | 1.75          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 13       | 1.75          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 13       | 1.75          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 15       | 1.75          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 15       | 1.75          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 15       | 1.75          |
| (1,2500) | 1:182:A:LYS:HG2  | 1:189:A:PHE:HE2 | 17       | 1.74          |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2  | 1        | 1.74          |
| (1,988)  | 1:85:A:GLU:HA    | 1:86:A:PHE:HE2  | 18       | 1.74          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 5        | 1.74          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 5        | 1.74          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 5        | 1.74          |
| (1,106)  | 1:19:A:LEU:HD21  | 1:22:A:PHE:HD1  | 11       | 1.74          |
| (1,106)  | 1:19:A:LEU:HD22  | 1:22:A:PHE:HD1  | 11       | 1.74          |
| (1,106)  | 1:19:A:LEU:HD23  | 1:22:A:PHE:HD1  | 11       | 1.74          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,106)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HD1  | 14       | 1.74          |
| (1,106)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HD1  | 14       | 1.74          |
| (1,106)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HD1  | 14       | 1.74          |
| (1,106)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HD1  | 20       | 1.74          |
| (1,106)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HD1  | 20       | 1.74          |
| (1,106)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HD1  | 20       | 1.74          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG2 | 3        | 1.73          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG3 | 3        | 1.73          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG2 | 11       | 1.73          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG3 | 11       | 1.73          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG2 | 18       | 1.73          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG3 | 18       | 1.73          |
| (1,978)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HE1  | 20       | 1.73          |
| (1,978)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HE1  | 20       | 1.73          |
| (1,978)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HE1  | 20       | 1.73          |
| (1,988)  | 1:85:A:GLU:HA   | 1:86:A:PHE:HE2  | 6        | 1.72          |
| (1,978)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HE1  | 8        | 1.72          |
| (1,978)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HE1  | 8        | 1.72          |
| (1,978)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HE1  | 8        | 1.72          |
| (1,116)  | 1:21:A:ARG:HG2  | 1:22:A:PHE:HE2  | 17       | 1.72          |
| (1,109)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HE1  | 20       | 1.72          |
| (1,109)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HE1  | 20       | 1.72          |
| (1,109)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HE1  | 20       | 1.72          |
| (1,106)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HD1  | 3        | 1.72          |
| (1,106)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HD1  | 3        | 1.72          |
| (1,106)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HD1  | 3        | 1.72          |
| (1,106)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HD1  | 16       | 1.72          |
| (1,106)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HD1  | 16       | 1.72          |
| (1,106)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HD1  | 16       | 1.72          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG2 | 2        | 1.71          |
| (1,2411) | 1:161:A:PHE:HE1 | 1:182:A:LYS:HG3 | 2        | 1.71          |
| (1,1640) | 1:138:A:SER:HA  | 1:140:A:PHE:HD2 | 15       | 1.71          |
| (1,106)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HD1  | 17       | 1.71          |
| (1,106)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HD1  | 17       | 1.71          |
| (1,106)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HD1  | 17       | 1.71          |
| (1,106)  | 1:19:A:LEU:HD21 | 1:22:A:PHE:HD1  | 18       | 1.71          |
| (1,106)  | 1:19:A:LEU:HD22 | 1:22:A:PHE:HD1  | 18       | 1.71          |
| (1,106)  | 1:19:A:LEU:HD23 | 1:22:A:PHE:HD1  | 18       | 1.71          |
| (1,1639) | 1:138:A:SER:HB3 | 1:140:A:PHE:HE2 | 16       | 1.7           |
| (1,2103) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HB  | 20       | 1.69          |
| (1,988)  | 1:85:A:GLU:HA   | 1:86:A:PHE:HE2  | 20       | 1.69          |
| (1,116)  | 1:21:A:ARG:HG2  | 1:22:A:PHE:HE2  | 4        | 1.69          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,116)  | 1:21:A:ARG:HG2  | 1:22:A:PHE:HE2   | 16       | 1.69          |
| (1,983)  | 1:68:A:TYR:HD2  | 1:86:A:PHE:HE1   | 12       | 1.68          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 16       | 1.67          |
| (1,116)  | 1:21:A:ARG:HG2  | 1:22:A:PHE:HE2   | 1        | 1.67          |
| (1,116)  | 1:21:A:ARG:HG2  | 1:22:A:PHE:HE2   | 20       | 1.67          |
| (1,1640) | 1:138:A:SER:HA  | 1:140:A:PHE:HD2  | 19       | 1.66          |
| (1,116)  | 1:21:A:ARG:HG2  | 1:22:A:PHE:HE2   | 2        | 1.66          |
| (1,116)  | 1:21:A:ARG:HG2  | 1:22:A:PHE:HE2   | 12       | 1.66          |
| (1,2103) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HB   | 7        | 1.65          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 17       | 1.65          |
| (1,116)  | 1:21:A:ARG:HG2  | 1:22:A:PHE:HE2   | 9        | 1.65          |
| (1,116)  | 1:21:A:ARG:HG2  | 1:22:A:PHE:HE2   | 13       | 1.65          |
| (1,112)  | 1:19:A:LEU:HA   | 1:22:A:PHE:HE1   | 9        | 1.65          |
| (1,988)  | 1:85:A:GLU:HA   | 1:86:A:PHE:HE2   | 12       | 1.64          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG11 | 11       | 1.63          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG12 | 11       | 1.63          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG13 | 11       | 1.63          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG21 | 11       | 1.63          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG22 | 11       | 1.63          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG23 | 11       | 1.63          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG11 | 16       | 1.63          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG12 | 16       | 1.63          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG13 | 16       | 1.63          |
| (1,1055) | 1:94:A:SER:HA   | 1:95:A:PHE:HE2   | 7        | 1.63          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 8        | 1.63          |
| (1,116)  | 1:21:A:ARG:HG2  | 1:22:A:PHE:HE2   | 19       | 1.63          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 1        | 1.62          |
| (1,116)  | 1:21:A:ARG:HG2  | 1:22:A:PHE:HE2   | 7        | 1.62          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG11 | 16       | 1.61          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG12 | 16       | 1.61          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG13 | 16       | 1.61          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG21 | 16       | 1.61          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG22 | 16       | 1.61          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG23 | 16       | 1.61          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG11 | 11       | 1.61          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG12 | 11       | 1.61          |
| (1,2101) | 1:142:A:TYR:HE1 | 1:167:A:VAL:HG13 | 11       | 1.61          |
| (1,1641) | 1:138:A:SER:HA  | 1:140:A:PHE:HE2  | 13       | 1.61          |
| (1,970)  | 1:25:A:ASP:H    | 1:86:A:PHE:HE2   | 12       | 1.61          |
| (1,1968) | 1:124:A:ALA:HB1 | 1:161:A:PHE:HD1  | 3        | 1.6           |
| (1,1968) | 1:124:A:ALA:HB2 | 1:161:A:PHE:HD1  | 3        | 1.6           |
| (1,1968) | 1:124:A:ALA:HB3 | 1:161:A:PHE:HD1  | 3        | 1.6           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,116)  | 1:21:A:ARG:HG2   | 1:22:A:PHE:HE2  | 8        | 1.6           |
| (1,112)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HE1  | 12       | 1.6           |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 17       | 1.59          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 17       | 1.59          |
| (1,112)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HE1  | 20       | 1.59          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 18       | 1.58          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1  | 18       | 1.58          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1  | 18       | 1.58          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 1        | 1.57          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 1        | 1.57          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 8        | 1.57          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 8        | 1.57          |
| (1,1668) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HD1 | 1        | 1.57          |
| (1,1668) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HD1 | 1        | 1.57          |
| (1,1668) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HD1 | 1        | 1.57          |
| (1,116)  | 1:21:A:ARG:HG2   | 1:22:A:PHE:HE2  | 11       | 1.57          |
| (1,1668) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HD1 | 18       | 1.56          |
| (1,1668) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HD1 | 18       | 1.56          |
| (1,1668) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HD1 | 18       | 1.56          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1  | 4        | 1.56          |
| (1,970)  | 1:25:A:ASP:H     | 1:86:A:PHE:HE2  | 19       | 1.56          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1 | 11       | 1.55          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1 | 11       | 1.55          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1 | 11       | 1.55          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2 | 16       | 1.55          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2 | 20       | 1.55          |
| (1,1646) | 1:139:A:LEU:HB2  | 1:140:A:PHE:HD2 | 16       | 1.55          |
| (1,1646) | 1:139:A:LEU:HB2  | 1:140:A:PHE:HD2 | 20       | 1.55          |
| (1,1645) | 1:139:A:LEU:HA   | 1:140:A:PHE:HD2 | 16       | 1.55          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1  | 12       | 1.55          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 1        | 1.55          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1  | 1        | 1.55          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1  | 1        | 1.55          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 5        | 1.54          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 5        | 1.54          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 19       | 1.54          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 19       | 1.54          |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2 | 2        | 1.54          |
| (1,1640) | 1:138:A:SER:HA   | 1:140:A:PHE:HD2 | 18       | 1.54          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 19       | 1.54          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1  | 19       | 1.54          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1  | 19       | 1.54          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,116)  | 1:21:A:ARG:HG2   | 1:22:A:PHE:HE2  | 14       | 1.54          |
| (1,2103) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HB  | 18       | 1.53          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 6        | 1.53          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 6        | 1.53          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1 | 1        | 1.53          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1 | 1        | 1.53          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1 | 1        | 1.53          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1 | 2        | 1.53          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1 | 2        | 1.53          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1 | 2        | 1.53          |
| (1,1645) | 1:139:A:LEU:HA   | 1:140:A:PHE:HD2 | 20       | 1.53          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1 | 18       | 1.52          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1 | 18       | 1.52          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1 | 18       | 1.52          |
| (1,1668) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HD1 | 20       | 1.52          |
| (1,1668) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HD1 | 20       | 1.52          |
| (1,1668) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HD1 | 20       | 1.52          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 16       | 1.52          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 16       | 1.52          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 5        | 1.52          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1  | 5        | 1.52          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1  | 5        | 1.52          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 6        | 1.52          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1  | 6        | 1.52          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1  | 6        | 1.52          |
| (1,970)  | 1:25:A:ASP:H     | 1:86:A:PHE:HE2  | 18       | 1.52          |
| (1,970)  | 1:25:A:ASP:H     | 1:86:A:PHE:HE2  | 20       | 1.52          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 16       | 1.51          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 16       | 1.51          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1 | 7        | 1.51          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1 | 7        | 1.51          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1 | 7        | 1.51          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 9        | 1.51          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1  | 9        | 1.51          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1  | 9        | 1.51          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 2        | 1.5           |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 2        | 1.5           |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 13       | 1.5           |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 13       | 1.5           |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 1        | 1.5           |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 1        | 1.5           |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 4        | 1.5           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,978)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HE1   | 4        | 1.5           |
| (1,978)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HE1   | 4        | 1.5           |
| (1,989)  | 1:85:A:GLU:HB2  | 1:86:A:PHE:HD2   | 8        | 1.49          |
| (1,989)  | 1:85:A:GLU:HB3  | 1:86:A:PHE:HD2   | 8        | 1.49          |
| (1,983)  | 1:68:A:TYR:HD2  | 1:86:A:PHE:HE1   | 1        | 1.49          |
| (1,978)  | 1:35:A:LEU:HD11 | 1:86:A:PHE:HE1   | 13       | 1.49          |
| (1,978)  | 1:35:A:LEU:HD12 | 1:86:A:PHE:HE1   | 13       | 1.49          |
| (1,978)  | 1:35:A:LEU:HD13 | 1:86:A:PHE:HE1   | 13       | 1.49          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG11 | 18       | 1.48          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG12 | 18       | 1.48          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG13 | 18       | 1.48          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG21 | 18       | 1.48          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG22 | 18       | 1.48          |
| (1,2106) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HG23 | 18       | 1.48          |
| (1,2010) | 1:161:A:PHE:HE2 | 1:163:A:MET:HG2  | 12       | 1.48          |
| (1,2010) | 1:161:A:PHE:HE2 | 1:163:A:MET:HG3  | 12       | 1.48          |
| (1,1968) | 1:124:A:ALA:HB1 | 1:161:A:PHE:HD1  | 4        | 1.48          |
| (1,1968) | 1:124:A:ALA:HB2 | 1:161:A:PHE:HD1  | 4        | 1.48          |
| (1,1968) | 1:124:A:ALA:HB3 | 1:161:A:PHE:HD1  | 4        | 1.48          |
| (1,1968) | 1:124:A:ALA:HB1 | 1:161:A:PHE:HD1  | 14       | 1.48          |
| (1,1968) | 1:124:A:ALA:HB2 | 1:161:A:PHE:HD1  | 14       | 1.48          |
| (1,1968) | 1:124:A:ALA:HB3 | 1:161:A:PHE:HD1  | 14       | 1.48          |
| (1,2010) | 1:161:A:PHE:HE2 | 1:163:A:MET:HG2  | 4        | 1.47          |
| (1,2010) | 1:161:A:PHE:HE2 | 1:163:A:MET:HG3  | 4        | 1.47          |
| (1,989)  | 1:85:A:GLU:HB2  | 1:86:A:PHE:HD2   | 4        | 1.47          |
| (1,989)  | 1:85:A:GLU:HB3  | 1:86:A:PHE:HD2   | 4        | 1.47          |
| (1,989)  | 1:85:A:GLU:HB2  | 1:86:A:PHE:HD2   | 17       | 1.47          |
| (1,989)  | 1:85:A:GLU:HB3  | 1:86:A:PHE:HD2   | 17       | 1.47          |
| (1,989)  | 1:85:A:GLU:HB2  | 1:86:A:PHE:HD2   | 19       | 1.47          |
| (1,989)  | 1:85:A:GLU:HB3  | 1:86:A:PHE:HD2   | 19       | 1.47          |
| (1,986)  | 1:70:A:ALA:HA   | 1:86:A:PHE:HD2   | 12       | 1.47          |
| (1,2010) | 1:161:A:PHE:HE2 | 1:163:A:MET:HG2  | 15       | 1.46          |
| (1,2010) | 1:161:A:PHE:HE2 | 1:163:A:MET:HG3  | 15       | 1.46          |
| (1,1968) | 1:124:A:ALA:HB1 | 1:161:A:PHE:HD1  | 10       | 1.46          |
| (1,1968) | 1:124:A:ALA:HB2 | 1:161:A:PHE:HD1  | 10       | 1.46          |
| (1,1968) | 1:124:A:ALA:HB3 | 1:161:A:PHE:HD1  | 10       | 1.46          |
| (1,1968) | 1:124:A:ALA:HB1 | 1:161:A:PHE:HD1  | 19       | 1.45          |
| (1,1968) | 1:124:A:ALA:HB2 | 1:161:A:PHE:HD1  | 19       | 1.45          |
| (1,1968) | 1:124:A:ALA:HB3 | 1:161:A:PHE:HD1  | 19       | 1.45          |
| (1,986)  | 1:70:A:ALA:HA   | 1:86:A:PHE:HD2   | 9        | 1.45          |
| (1,2696) | 1:142:A:TYR:HE1 | 1:196:A:LEU:HD11 | 1        | 1.44          |
| (1,2696) | 1:142:A:TYR:HE1 | 1:196:A:LEU:HD12 | 1        | 1.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD13 | 1        | 1.44          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD21 | 1        | 1.44          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD22 | 1        | 1.44          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD23 | 1        | 1.44          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2  | 11       | 1.44          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3  | 11       | 1.44          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1  | 16       | 1.44          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1  | 16       | 1.44          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1  | 16       | 1.44          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 8        | 1.44          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1   | 11       | 1.44          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1   | 11       | 1.44          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1   | 11       | 1.44          |
| (1,116)  | 1:21:A:ARG:HG2   | 1:22:A:PHE:HE2   | 10       | 1.44          |
| (1,1640) | 1:138:A:SER:HA   | 1:140:A:PHE:HD2  | 10       | 1.43          |
| (1,1639) | 1:138:A:SER:HB3  | 1:140:A:PHE:HE2  | 3        | 1.43          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2   | 3        | 1.43          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2   | 3        | 1.43          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2   | 18       | 1.43          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2   | 18       | 1.43          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1   | 14       | 1.43          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1   | 14       | 1.43          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1   | 14       | 1.43          |
| (1,116)  | 1:21:A:ARG:HG2   | 1:22:A:PHE:HE2   | 5        | 1.43          |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG11 | 7        | 1.42          |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG12 | 7        | 1.42          |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG13 | 7        | 1.42          |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG21 | 7        | 1.42          |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG22 | 7        | 1.42          |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG23 | 7        | 1.42          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2  | 3        | 1.42          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3  | 3        | 1.42          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1  | 6        | 1.42          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1  | 6        | 1.42          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1  | 6        | 1.42          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1  | 13       | 1.42          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1  | 13       | 1.42          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1  | 13       | 1.42          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2  | 16       | 1.42          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2  | 16       | 1.42          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2  | 16       | 1.42          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2  | 17       | 1.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2  | 17       | 1.42          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2  | 17       | 1.42          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2  | 2        | 1.42          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2   | 7        | 1.42          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2   | 20       | 1.42          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1   | 10       | 1.42          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1   | 10       | 1.42          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1   | 10       | 1.42          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1   | 15       | 1.42          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1   | 15       | 1.42          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1   | 15       | 1.42          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2  | 7        | 1.41          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3  | 7        | 1.41          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2  | 18       | 1.41          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3  | 18       | 1.41          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1  | 15       | 1.41          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1  | 15       | 1.41          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1  | 15       | 1.41          |
| (1,1638) | 1:138:A:SER:HB2  | 1:140:A:PHE:HE2  | 18       | 1.41          |
| (1,116)  | 1:21:A:ARG:HG2   | 1:22:A:PHE:HE2   | 6        | 1.41          |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG11 | 20       | 1.4           |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG12 | 20       | 1.4           |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG13 | 20       | 1.4           |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG21 | 20       | 1.4           |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG22 | 20       | 1.4           |
| (1,2106) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HG23 | 20       | 1.4           |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2  | 14       | 1.4           |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3  | 14       | 1.4           |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2  | 20       | 1.4           |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3  | 20       | 1.4           |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1  | 17       | 1.4           |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1  | 17       | 1.4           |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1  | 17       | 1.4           |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2  | 2        | 1.4           |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2  | 2        | 1.4           |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2  | 2        | 1.4           |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2   | 20       | 1.4           |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2   | 20       | 1.4           |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2   | 1        | 1.4           |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2   | 6        | 1.4           |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2   | 11       | 1.4           |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2   | 14       | 1.4           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1  | 5        | 1.4           |
| (1,116)  | 1:21:A:ARG:HG2   | 1:22:A:PHE:HE2  | 15       | 1.4           |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 7        | 1.4           |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 10       | 1.4           |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1 | 20       | 1.39          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1 | 20       | 1.39          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1 | 20       | 1.39          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 18       | 1.39          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 18       | 1.39          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 18       | 1.39          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 16       | 1.39          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 16       | 1.39          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 16       | 1.39          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 16       | 1.39          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 16       | 1.39          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 16       | 1.39          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 5        | 1.39          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 10       | 1.39          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 13       | 1.39          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1  | 4        | 1.39          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 1        | 1.39          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 3        | 1.39          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 11       | 1.39          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 13       | 1.39          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 10       | 1.38          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 10       | 1.38          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1 | 9        | 1.38          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1 | 9        | 1.38          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1 | 9        | 1.38          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 20       | 1.38          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 20       | 1.38          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 20       | 1.38          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 20       | 1.38          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 20       | 1.38          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 20       | 1.38          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 2        | 1.38          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 8        | 1.38          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 15       | 1.38          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 18       | 1.38          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 19       | 1.38          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 17       | 1.38          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1  | 17       | 1.38          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1  | 17       | 1.38          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1 | 12       | 1.37          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1 | 12       | 1.37          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1 | 12       | 1.37          |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2 | 14       | 1.37          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 13       | 1.37          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 13       | 1.37          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG2 | 9        | 1.36          |
| (1,2010) | 1:161:A:PHE:HE2  | 1:163:A:MET:HG3 | 9        | 1.36          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1 | 5        | 1.36          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1 | 5        | 1.36          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1 | 5        | 1.36          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 5        | 1.36          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 5        | 1.36          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 5        | 1.36          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 2        | 1.36          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 2        | 1.36          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 2        | 1.36          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 16       | 1.36          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 16       | 1.36          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 16       | 1.36          |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2 | 17       | 1.36          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 9        | 1.36          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 9        | 1.36          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 12       | 1.36          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 12       | 1.36          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 17       | 1.36          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 4        | 1.36          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 17       | 1.36          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 10       | 1.35          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 10       | 1.35          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 10       | 1.35          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 3        | 1.35          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1  | 13       | 1.35          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 16       | 1.35          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1  | 16       | 1.35          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1  | 16       | 1.35          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 19       | 1.35          |
| (1,2103) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HB  | 16       | 1.34          |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2 | 11       | 1.34          |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2 | 15       | 1.34          |
| (1,1640) | 1:138:A:SER:HA   | 1:140:A:PHE:HD2 | 3        | 1.34          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 2        | 1.34          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 2        | 1.34          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 5        | 1.34          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 5        | 1.34          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 10       | 1.34          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 10       | 1.34          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1  | 1        | 1.34          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 7        | 1.34          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1  | 7        | 1.34          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1  | 7        | 1.34          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 18       | 1.34          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 1        | 1.33          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 1        | 1.33          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 1        | 1.33          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 7        | 1.33          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 7        | 1.33          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 7        | 1.33          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 9        | 1.33          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 9        | 1.33          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 9        | 1.33          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 12       | 1.33          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 12       | 1.33          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 12       | 1.33          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 13       | 1.33          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 13       | 1.33          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 13       | 1.33          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 13       | 1.33          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 13       | 1.33          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 13       | 1.33          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 15       | 1.33          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 15       | 1.33          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 4        | 1.33          |
| (1,986)  | 1:70:A:ALA:HA    | 1:86:A:PHE:HD2  | 16       | 1.33          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 2        | 1.33          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 2        | 1.32          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 4        | 1.32          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 11       | 1.32          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 13       | 1.32          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 18       | 1.32          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 3        | 1.32          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 3        | 1.32          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 3        | 1.32          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 8        | 1.32          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 8        | 1.32          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 8        | 1.32          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 11       | 1.32          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 11       | 1.32          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 11       | 1.32          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 1        | 1.32          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 1        | 1.32          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 1        | 1.32          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 11       | 1.32          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 11       | 1.32          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 11       | 1.32          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 11       | 1.32          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 11       | 1.32          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 14       | 1.32          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 14       | 1.32          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 16       | 1.32          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 3        | 1.31          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 14       | 1.31          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 6        | 1.31          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 6        | 1.31          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 6        | 1.31          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 4        | 1.31          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 4        | 1.31          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 4        | 1.31          |
| (1,1675) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HE2 | 20       | 1.31          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1  | 6        | 1.31          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 5        | 1.31          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 6        | 1.31          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 1        | 1.3           |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 6        | 1.3           |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 10       | 1.3           |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 15       | 1.3           |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 16       | 1.3           |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 4        | 1.3           |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 4        | 1.3           |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 4        | 1.3           |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 14       | 1.3           |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 14       | 1.3           |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 14       | 1.3           |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 20       | 1.3           |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 20       | 1.3           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 20       | 1.3           |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 9        | 1.3           |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 9        | 1.3           |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 9        | 1.3           |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2 | 17       | 1.3           |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 9        | 1.29          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 12       | 1.29          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 17       | 1.29          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 17       | 1.29          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 17       | 1.29          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1  | 5        | 1.29          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1  | 8        | 1.29          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1  | 3        | 1.29          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1  | 3        | 1.29          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1  | 3        | 1.29          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1  | 18       | 1.29          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1  | 18       | 1.29          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 19       | 1.28          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 3        | 1.28          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 3        | 1.28          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 3        | 1.28          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 18       | 1.28          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 18       | 1.28          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 18       | 1.28          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2 | 11       | 1.28          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 6        | 1.28          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 6        | 1.28          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1  | 19       | 1.28          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1  | 19       | 1.28          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 5        | 1.27          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 7        | 1.27          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 12       | 1.27          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 12       | 1.27          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 12       | 1.27          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2 | 14       | 1.27          |
| (1,989)  | 1:85:A:GLU:HB2   | 1:86:A:PHE:HD2  | 7        | 1.27          |
| (1,989)  | 1:85:A:GLU:HB3   | 1:86:A:PHE:HD2  | 7        | 1.27          |
| (1,104)  | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 20       | 1.27          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 17       | 1.26          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 20       | 1.26          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 15       | 1.26          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 15       | 1.26          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 15       | 1.26          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 5        | 1.26          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 5        | 1.26          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 5        | 1.26          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 6        | 1.26          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 6        | 1.26          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 6        | 1.26          |
| (1,1986) | 1:161:A:PHE:HA   | 1:161:A:PHE:HD2 | 8        | 1.25          |
| (1,1966) | 1:114:A:VAL:HG21 | 1:161:A:PHE:HE2 | 19       | 1.25          |
| (1,1966) | 1:114:A:VAL:HG22 | 1:161:A:PHE:HE2 | 19       | 1.25          |
| (1,1966) | 1:114:A:VAL:HG23 | 1:161:A:PHE:HE2 | 19       | 1.25          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 10       | 1.25          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 10       | 1.25          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 10       | 1.25          |
| (1,1987) | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2  | 6        | 1.25          |
| (1,1987) | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2  | 6        | 1.25          |
| (1,1987) | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2  | 6        | 1.25          |
| (1,1104) | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 8        | 1.25          |
| (1,1104) | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 14       | 1.25          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 15       | 1.24          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 15       | 1.24          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 15       | 1.24          |
| (1,1104) | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 9        | 1.24          |
| (1,1104) | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 15       | 1.24          |
| (1,1968) | 1:124:A:ALA:HB1  | 1:161:A:PHE:HD1 | 8        | 1.23          |
| (1,1968) | 1:124:A:ALA:HB2  | 1:161:A:PHE:HD1 | 8        | 1.23          |
| (1,1968) | 1:124:A:ALA:HB3  | 1:161:A:PHE:HD1 | 8        | 1.23          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 7        | 1.23          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 7        | 1.23          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 7        | 1.23          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 14       | 1.23          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 14       | 1.23          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 14       | 1.23          |
| (1,1987) | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2  | 5        | 1.23          |
| (1,1987) | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2  | 5        | 1.23          |
| (1,1987) | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2  | 5        | 1.23          |
| (1,1104) | 1:19:A:LEU:HA    | 1:22:A:PHE:HD1  | 12       | 1.23          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2 | 20       | 1.22          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2 | 20       | 1.22          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2 | 20       | 1.22          |
| (1,1987) | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2  | 9        | 1.22          |
| (1,1987) | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2  | 9        | 1.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 9        | 1.22          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 20       | 1.22          |
| (1,978)  | 1:35:A:LEU:HD11  | 1:86:A:PHE:HE1   | 2        | 1.22          |
| (1,978)  | 1:35:A:LEU:HD12  | 1:86:A:PHE:HE1   | 2        | 1.22          |
| (1,978)  | 1:35:A:LEU:HD13  | 1:86:A:PHE:HE1   | 2        | 1.22          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD11 | 16       | 1.21          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD12 | 16       | 1.21          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD13 | 16       | 1.21          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD21 | 16       | 1.21          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD22 | 16       | 1.21          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD23 | 16       | 1.21          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 2        | 1.21          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 3        | 1.21          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 4        | 1.21          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 11       | 1.21          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 13       | 1.21          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 18       | 1.21          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2  | 13       | 1.21          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2  | 15       | 1.21          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 10       | 1.21          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 10       | 1.21          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 10       | 1.21          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1   | 6        | 1.21          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1   | 13       | 1.21          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 1        | 1.2           |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 6        | 1.2           |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 10       | 1.2           |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 14       | 1.2           |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 15       | 1.2           |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 16       | 1.2           |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2  | 19       | 1.2           |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2  | 19       | 1.2           |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2  | 19       | 1.2           |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2  | 19       | 1.2           |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 7        | 1.2           |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 7        | 1.2           |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 7        | 1.2           |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 11       | 1.2           |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 11       | 1.2           |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 11       | 1.2           |
| (1,2103) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HB   | 1        | 1.19          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 9        | 1.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 12       | 1.19          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 16       | 1.19          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 17       | 1.19          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 5        | 1.18          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 7        | 1.18          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 19       | 1.18          |
| (1,1963) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HD2  | 8        | 1.18          |
| (1,1963) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HD2  | 8        | 1.18          |
| (1,1963) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HD2  | 8        | 1.18          |
| (1,1639) | 1:138:A:SER:HB3  | 1:140:A:PHE:HE2  | 19       | 1.18          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 13       | 1.18          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 13       | 1.18          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 13       | 1.18          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 15       | 1.18          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 15       | 1.18          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 15       | 1.18          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 20       | 1.17          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 14       | 1.17          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 14       | 1.17          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 14       | 1.17          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD11 | 11       | 1.16          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD12 | 11       | 1.16          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD13 | 11       | 1.16          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD21 | 11       | 1.16          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD22 | 11       | 1.16          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD23 | 11       | 1.16          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 17       | 1.16          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2  | 2        | 1.16          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2  | 2        | 1.16          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2  | 2        | 1.16          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2  | 19       | 1.16          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 9        | 1.16          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 10       | 1.16          |
| (1,1987) | 1:161:A:PHE:HA   | 1:161:A:PHE:HE2  | 8        | 1.15          |
| (1,1675) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HE2  | 16       | 1.15          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 12       | 1.15          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 12       | 1.15          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 12       | 1.15          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2  | 11       | 1.14          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2  | 11       | 1.14          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2  | 11       | 1.14          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2  | 13       | 1.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2 | 13       | 1.14          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2 | 13       | 1.14          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 8        | 1.14          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 8        | 1.14          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 8        | 1.14          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 8        | 1.14          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 8        | 1.14          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 8        | 1.14          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2  | 2        | 1.14          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2  | 2        | 1.14          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2  | 2        | 1.14          |
| (1,2103) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HB  | 11       | 1.13          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2 | 16       | 1.13          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2 | 16       | 1.13          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2 | 16       | 1.13          |
| (1,1639) | 1:138:A:SER:HB3  | 1:140:A:PHE:HE2 | 10       | 1.13          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2 | 1        | 1.12          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2 | 1        | 1.12          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2 | 1        | 1.12          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2 | 4        | 1.12          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2 | 4        | 1.12          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2 | 4        | 1.12          |
| (1,2493) | 1:182:A:LYS:HE3  | 1:189:A:PHE:HE2 | 17       | 1.11          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 6        | 1.11          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 6        | 1.11          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 6        | 1.11          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 6        | 1.11          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 6        | 1.11          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 6        | 1.11          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2  | 3        | 1.11          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2  | 3        | 1.11          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2  | 3        | 1.11          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1  | 3        | 1.11          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2 | 3        | 1.1           |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2 | 3        | 1.1           |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2 | 3        | 1.1           |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 5        | 1.1           |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 5        | 1.1           |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 5        | 1.1           |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 5        | 1.1           |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 5        | 1.1           |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 5        | 1.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 7        | 1.1           |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 11       | 1.1           |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2  | 9        | 1.09          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2  | 9        | 1.09          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2  | 9        | 1.09          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2  | 4        | 1.09          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2  | 4        | 1.09          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2  | 4        | 1.09          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2  | 4        | 1.09          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2  | 4        | 1.09          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2  | 4        | 1.09          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2  | 12       | 1.09          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2  | 12       | 1.09          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2  | 12       | 1.09          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2  | 12       | 1.09          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2  | 12       | 1.09          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2  | 12       | 1.09          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 16       | 1.08          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 16       | 1.08          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 16       | 1.08          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2  | 2        | 1.07          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2  | 2        | 1.07          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2  | 2        | 1.07          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2  | 2        | 1.07          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2  | 2        | 1.07          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2  | 2        | 1.07          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 4        | 1.07          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 4        | 1.07          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 4        | 1.07          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD11 | 20       | 1.06          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD12 | 20       | 1.06          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD13 | 20       | 1.06          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD21 | 20       | 1.06          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD22 | 20       | 1.06          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD23 | 20       | 1.06          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2  | 12       | 1.06          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2  | 12       | 1.06          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2  | 12       | 1.06          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2  | 18       | 1.06          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2  | 18       | 1.06          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2  | 18       | 1.06          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2  | 18       | 1.06          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 9        | 1.06          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 9        | 1.06          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 9        | 1.06          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 9        | 1.06          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 9        | 1.06          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 9        | 1.06          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1  | 14       | 1.06          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1  | 14       | 1.06          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2 | 17       | 1.05          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2 | 17       | 1.05          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2 | 17       | 1.05          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2 | 10       | 1.04          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2 | 10       | 1.04          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2 | 10       | 1.04          |
| (1,1639) | 1:138:A:SER:HB3  | 1:140:A:PHE:HE2 | 20       | 1.04          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2  | 8        | 1.04          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2  | 8        | 1.04          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2  | 8        | 1.04          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1  | 9        | 1.04          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1  | 10       | 1.04          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1  | 20       | 1.04          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1  | 20       | 1.04          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2 | 6        | 1.03          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2 | 6        | 1.03          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2 | 6        | 1.03          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2  | 20       | 1.03          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2  | 20       | 1.03          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2  | 20       | 1.03          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1  | 16       | 1.03          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2 | 5        | 1.02          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2 | 5        | 1.02          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2 | 5        | 1.02          |
| (1,1677) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HD2 | 20       | 1.02          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2 | 10       | 1.02          |
| (1,1055) | 1:94:A:SER:HA    | 1:95:A:PHE:HE2  | 13       | 1.02          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1  | 18       | 1.02          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1  | 10       | 1.02          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1  | 10       | 1.02          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2 | 7        | 1.01          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2 | 7        | 1.01          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2 | 7        | 1.01          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2 | 14       | 1.01          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2  | 14       | 1.01          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2  | 14       | 1.01          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2  | 15       | 1.01          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2  | 15       | 1.01          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2  | 15       | 1.01          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 17       | 1.01          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 17       | 1.01          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 17       | 1.01          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 19       | 1.01          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 15       | 1.01          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 15       | 1.01          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1   | 17       | 1.0           |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 2        | 1.0           |
| (1,2510) | 1:183:A:SER:H    | 1:189:A:PHE:HD2  | 17       | 0.99          |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2  | 18       | 0.99          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 1        | 0.99          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 1        | 0.99          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 1        | 0.99          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1   | 3        | 0.99          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 15       | 0.99          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2  | 20       | 0.97          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2  | 20       | 0.97          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2  | 20       | 0.97          |
| (1,1666) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HE1  | 11       | 0.97          |
| (1,1666) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HE1  | 11       | 0.97          |
| (1,1666) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HE1  | 11       | 0.97          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 19       | 0.97          |
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 19       | 0.97          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 19       | 0.97          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1   | 11       | 0.97          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 13       | 0.97          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 13       | 0.97          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG21 | 1        | 0.96          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG22 | 1        | 0.96          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG23 | 1        | 0.96          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2  | 19       | 0.96          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2  | 19       | 0.96          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2  | 19       | 0.96          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1   | 7        | 0.96          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 17       | 0.96          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 20       | 0.96          |
| (1,987)  | 1:70:A:ALA:HB1   | 1:86:A:PHE:HD2   | 18       | 0.95          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,987)  | 1:70:A:ALA:HB2   | 1:86:A:PHE:HD2   | 18       | 0.95          |
| (1,987)  | 1:70:A:ALA:HB3   | 1:86:A:PHE:HD2   | 18       | 0.95          |
| (1,983)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HE1   | 14       | 0.95          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 11       | 0.95          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 11       | 0.95          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 16       | 0.95          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 16       | 0.95          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 3        | 0.95          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 12       | 0.95          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 16       | 0.95          |
| (1,2506) | 1:182:A:LYS:HG2  | 1:189:A:PHE:HD2  | 17       | 0.94          |
| (1,2506) | 1:182:A:LYS:HG3  | 1:189:A:PHE:HD2  | 17       | 0.94          |
| (1,1965) | 1:114:A:VAL:HG11 | 1:161:A:PHE:HE2  | 8        | 0.94          |
| (1,1965) | 1:114:A:VAL:HG12 | 1:161:A:PHE:HE2  | 8        | 0.94          |
| (1,1965) | 1:114:A:VAL:HG13 | 1:161:A:PHE:HE2  | 8        | 0.94          |
| (1,1651) | 1:140:A:PHE:H    | 1:140:A:PHE:HD2  | 3        | 0.94          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 9        | 0.94          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 18       | 0.94          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 19       | 0.94          |
| (1,1677) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HD2  | 16       | 0.93          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 9        | 0.93          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 9        | 0.93          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 4        | 0.93          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 8        | 0.92          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 13       | 0.92          |
| (1,2466) | 1:124:A:ALA:H    | 1:189:A:PHE:HE1  | 17       | 0.91          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 6        | 0.91          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 6        | 0.91          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 1        | 0.91          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 2        | 0.91          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1   | 2        | 0.9           |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1   | 20       | 0.9           |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11  | 12       | 0.9           |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12  | 12       | 0.9           |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13  | 12       | 0.9           |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21  | 12       | 0.9           |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22  | 12       | 0.9           |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23  | 12       | 0.9           |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD11 | 7        | 0.89          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD12 | 7        | 0.89          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD13 | 7        | 0.89          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD21 | 7        | 0.89          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD22 | 7        | 0.89          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD23 | 7        | 0.89          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD11 | 18       | 0.89          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD12 | 18       | 0.89          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD13 | 18       | 0.89          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD21 | 18       | 0.89          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD22 | 18       | 0.89          |
| (1,2696) | 1:142:A:TYR:HE1  | 1:196:A:LEU:HD23 | 18       | 0.89          |
| (1,1666) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HE1  | 16       | 0.89          |
| (1,1666) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HE1  | 16       | 0.89          |
| (1,1666) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HE1  | 16       | 0.89          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 7        | 0.89          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 14       | 0.89          |
| (1,1055) | 1:94:A:SER:HA    | 1:95:A:PHE:HE2   | 1        | 0.88          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 11       | 0.88          |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2  | 10       | 0.87          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 5        | 0.87          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 5        | 0.87          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 7        | 0.87          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 7        | 0.87          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 10       | 0.87          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 15       | 0.87          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG21 | 16       | 0.86          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG22 | 16       | 0.86          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG23 | 16       | 0.86          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2  | 15       | 0.86          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2  | 15       | 0.86          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2  | 15       | 0.86          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2  | 15       | 0.86          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2  | 15       | 0.86          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2  | 15       | 0.86          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1   | 15       | 0.86          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 5        | 0.86          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG21 | 7        | 0.85          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG22 | 7        | 0.85          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG23 | 7        | 0.85          |
| (1,124)  | 1:22:A:PHE:H     | 1:22:A:PHE:HE2   | 6        | 0.85          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1   | 18       | 0.84          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 3        | 0.83          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 3        | 0.83          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 8        | 0.83          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 8        | 0.83          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1  | 19       | 0.82          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1  | 1        | 0.82          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1  | 1        | 0.82          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 2        | 0.81          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 2        | 0.81          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 2        | 0.81          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 19       | 0.81          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 19       | 0.81          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 19       | 0.81          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 19       | 0.81          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 19       | 0.81          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 19       | 0.81          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2  | 18       | 0.81          |
| (1,984)  | 1:68:A:TYR:HD2   | 1:86:A:PHE:HD1  | 14       | 0.81          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1  | 17       | 0.81          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1  | 17       | 0.81          |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1  | 20       | 0.81          |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1  | 20       | 0.81          |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1  | 20       | 0.81          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 8        | 0.81          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 8        | 0.81          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 8        | 0.81          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 8        | 0.81          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 8        | 0.81          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 8        | 0.81          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 18       | 0.8           |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 18       | 0.8           |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 18       | 0.8           |
| (1,1675) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HE2 | 18       | 0.8           |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2  | 20       | 0.8           |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1  | 4        | 0.8           |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1  | 4        | 0.8           |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 9        | 0.79          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 9        | 0.79          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 9        | 0.79          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 9        | 0.79          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 9        | 0.79          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 9        | 0.79          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 16       | 0.78          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 16       | 0.78          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 16       | 0.78          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2  | 19       | 0.78          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 12       | 0.78          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 12       | 0.78          |
| (1,974)  | 1:32:A:ASN:HD21  | 1:86:A:PHE:HE1   | 2        | 0.77          |
| (1,974)  | 1:32:A:ASN:HD22  | 1:86:A:PHE:HE1   | 2        | 0.77          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2  | 17       | 0.76          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2  | 17       | 0.76          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2  | 17       | 0.76          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2  | 17       | 0.76          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2  | 17       | 0.76          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2  | 17       | 0.76          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11  | 4        | 0.76          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12  | 4        | 0.76          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13  | 4        | 0.76          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21  | 4        | 0.76          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22  | 4        | 0.76          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23  | 4        | 0.76          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2  | 6        | 0.75          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2  | 6        | 0.75          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2  | 6        | 0.75          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG21 | 20       | 0.74          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG22 | 20       | 0.74          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG23 | 20       | 0.74          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11  | 16       | 0.74          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12  | 16       | 0.74          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13  | 16       | 0.74          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21  | 16       | 0.74          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22  | 16       | 0.74          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23  | 16       | 0.74          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2  | 19       | 0.73          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2  | 19       | 0.73          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2  | 19       | 0.73          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2  | 14       | 0.73          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2  | 14       | 0.73          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2  | 14       | 0.73          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2  | 14       | 0.73          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2  | 14       | 0.73          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2  | 14       | 0.73          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2  | 4        | 0.72          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2  | 4        | 0.72          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2  | 4        | 0.72          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2  | 11       | 0.72          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2  | 11       | 0.72          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 11       | 0.72          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 11       | 0.72          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 11       | 0.72          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 11       | 0.72          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 20       | 0.72          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 20       | 0.72          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 20       | 0.72          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 20       | 0.72          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 20       | 0.72          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 20       | 0.72          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 5        | 0.71          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 5        | 0.71          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 5        | 0.71          |
| (1,1666) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HE1 | 7        | 0.71          |
| (1,1666) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HE1 | 7        | 0.71          |
| (1,1666) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HE1 | 7        | 0.71          |
| (1,2497) | 1:182:A:LYS:HD2  | 1:189:A:PHE:HE2 | 17       | 0.7           |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 11       | 0.7           |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 11       | 0.7           |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 11       | 0.7           |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 13       | 0.7           |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 13       | 0.7           |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 13       | 0.7           |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 17       | 0.7           |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 17       | 0.7           |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 17       | 0.7           |
| (1,1641) | 1:138:A:SER:HA   | 1:140:A:PHE:HE2 | 3        | 0.7           |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2  | 1        | 0.7           |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 3        | 0.69          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 3        | 0.69          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 3        | 0.69          |
| (1,1666) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HE1 | 1        | 0.69          |
| (1,1666) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HE1 | 1        | 0.69          |
| (1,1666) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HE1 | 1        | 0.69          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 13       | 0.69          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 13       | 0.69          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 13       | 0.69          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 13       | 0.69          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 13       | 0.69          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 13       | 0.69          |
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 1        | 0.69          |
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 6        | 0.69          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 13       | 0.69          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2  | 13       | 0.69          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2  | 17       | 0.69          |
| (1,2519) | 1:189:A:PHE:HB3  | 1:189:A:PHE:HE2 | 17       | 0.68          |
| (1,2508) | 1:182:A:LYS:HE2  | 1:189:A:PHE:HE2 | 17       | 0.68          |
| (1,2508) | 1:182:A:LYS:HE3  | 1:189:A:PHE:HE2 | 17       | 0.68          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 1        | 0.68          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 1        | 0.68          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 1        | 0.68          |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 18       | 0.67          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 18       | 0.67          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 18       | 0.67          |
| (1,965)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HE1  | 20       | 0.67          |
| (1,965)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HE1  | 20       | 0.67          |
| (1,965)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HE1  | 20       | 0.67          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 17       | 0.67          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 17       | 0.67          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 17       | 0.67          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 17       | 0.67          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 17       | 0.67          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 17       | 0.67          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 14       | 0.66          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 14       | 0.66          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 14       | 0.66          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 7        | 0.66          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 7        | 0.66          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 7        | 0.66          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 7        | 0.66          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 7        | 0.66          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 7        | 0.66          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2  | 7        | 0.66          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2  | 11       | 0.66          |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1  | 18       | 0.66          |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1  | 18       | 0.66          |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1  | 18       | 0.66          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 9        | 0.65          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 9        | 0.65          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 9        | 0.65          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 15       | 0.65          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 15       | 0.65          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 15       | 0.65          |
| (1,1677) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HD2 | 18       | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2   | 17       | 0.65          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 8        | 0.65          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 9        | 0.65          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 12       | 0.65          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG21 | 11       | 0.64          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG22 | 11       | 0.64          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG23 | 11       | 0.64          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2  | 10       | 0.64          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2  | 10       | 0.64          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2  | 10       | 0.64          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2  | 12       | 0.64          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2  | 12       | 0.64          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2  | 12       | 0.64          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 14       | 0.64          |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1   | 20       | 0.64          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1   | 20       | 0.64          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1   | 20       | 0.64          |
| (1,2104) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HB   | 1        | 0.63          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 16       | 0.63          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11  | 1        | 0.63          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12  | 1        | 0.63          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13  | 1        | 0.63          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21  | 1        | 0.63          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22  | 1        | 0.63          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23  | 1        | 0.63          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2  | 1        | 0.62          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2  | 1        | 0.62          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2  | 1        | 0.62          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2  | 1        | 0.62          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2  | 1        | 0.62          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2  | 1        | 0.62          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 2        | 0.62          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 3        | 0.62          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 4        | 0.62          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 10       | 0.62          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 15       | 0.62          |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1   | 19       | 0.62          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1   | 19       | 0.62          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1   | 19       | 0.62          |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1   | 12       | 0.62          |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1   | 12       | 0.62          |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1   | 12       | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1   | 17       | 0.62          |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1   | 17       | 0.62          |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1   | 17       | 0.62          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2  | 7        | 0.61          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2  | 7        | 0.61          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2  | 7        | 0.61          |
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2   | 18       | 0.61          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 5        | 0.61          |
| (1,993)  | 1:86:A:PHE:HA    | 1:86:A:PHE:HD2   | 6        | 0.61          |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1   | 8        | 0.61          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1   | 8        | 0.61          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1   | 8        | 0.61          |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1   | 19       | 0.61          |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1   | 19       | 0.61          |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1   | 19       | 0.61          |
| (1,965)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HE1   | 18       | 0.61          |
| (1,965)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HE1   | 18       | 0.61          |
| (1,965)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HE1   | 18       | 0.61          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11  | 18       | 0.61          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12  | 18       | 0.61          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13  | 18       | 0.61          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21  | 18       | 0.61          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22  | 18       | 0.61          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23  | 18       | 0.61          |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1   | 8        | 0.6           |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1   | 8        | 0.6           |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1   | 8        | 0.6           |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG21 | 18       | 0.59          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG22 | 18       | 0.59          |
| (1,2102) | 1:142:A:TYR:HE1  | 1:167:A:VAL:HG23 | 18       | 0.59          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2  | 10       | 0.59          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2  | 10       | 0.59          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2  | 10       | 0.59          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2  | 10       | 0.59          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2  | 10       | 0.59          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2  | 10       | 0.59          |
| (1,965)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HE1   | 19       | 0.59          |
| (1,965)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HE1   | 19       | 0.59          |
| (1,965)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HE1   | 19       | 0.59          |
| (1,1666) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HE1  | 18       | 0.58          |
| (1,1666) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HE1  | 18       | 0.58          |
| (1,1666) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HE1  | 18       | 0.58          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 1        | 0.58          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 1        | 0.58          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 1        | 0.58          |
| (1,2104) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HB  | 18       | 0.57          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 8        | 0.57          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 8        | 0.57          |
| (1,1675) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HE2 | 1        | 0.57          |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1  | 1        | 0.57          |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1  | 1        | 0.57          |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1  | 1        | 0.57          |
| (1,965)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HE1  | 12       | 0.57          |
| (1,965)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HE1  | 12       | 0.57          |
| (1,965)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HE1  | 12       | 0.57          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 17       | 0.56          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 17       | 0.56          |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 17       | 0.56          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 17       | 0.56          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 17       | 0.56          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 20       | 0.55          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 20       | 0.55          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 20       | 0.55          |
| (1,1666) | 1:129:A:ILE:HG21 | 1:142:A:TYR:HE1 | 20       | 0.55          |
| (1,1666) | 1:129:A:ILE:HG22 | 1:142:A:TYR:HE1 | 20       | 0.55          |
| (1,1666) | 1:129:A:ILE:HG23 | 1:142:A:TYR:HE1 | 20       | 0.55          |
| (1,1055) | 1:94:A:SER:HA    | 1:95:A:PHE:HE2  | 17       | 0.55          |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 12       | 0.55          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 12       | 0.55          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 12       | 0.55          |
| (1,965)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HE1  | 8        | 0.54          |
| (1,965)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HE1  | 8        | 0.54          |
| (1,965)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HE1  | 8        | 0.54          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 14       | 0.54          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 14       | 0.54          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 14       | 0.54          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 14       | 0.54          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 14       | 0.54          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 14       | 0.54          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 19       | 0.54          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 19       | 0.54          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 19       | 0.54          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 19       | 0.54          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 19       | 0.54          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 19       | 0.54          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 5        | 0.53          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 5        | 0.53          |
| (1,1675) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HE2 | 11       | 0.53          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 20       | 0.53          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 20       | 0.53          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 20       | 0.53          |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 20       | 0.53          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 20       | 0.53          |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 20       | 0.53          |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1  | 16       | 0.53          |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1  | 16       | 0.53          |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1  | 16       | 0.53          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 16       | 0.52          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 16       | 0.52          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 16       | 0.52          |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 16       | 0.52          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 16       | 0.52          |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 16       | 0.52          |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 16       | 0.52          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 16       | 0.52          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 16       | 0.52          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 13       | 0.52          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 13       | 0.52          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 13       | 0.52          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 13       | 0.52          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 13       | 0.52          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 13       | 0.52          |
| (1,965)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HE1  | 17       | 0.51          |
| (1,965)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HE1  | 17       | 0.51          |
| (1,965)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HE1  | 17       | 0.51          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 15       | 0.51          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 15       | 0.51          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 15       | 0.51          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 15       | 0.51          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 15       | 0.51          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 15       | 0.51          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 1        | 0.5           |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 1        | 0.5           |
| (1,1687) | 1:142:A:TYR:HB3  | 1:142:A:TYR:HD2 | 11       | 0.5           |
| (1,1687) | 1:142:A:TYR:HB3  | 1:142:A:TYR:HD2 | 18       | 0.5           |
| (1,973)  | 1:27:A:HIS:HD2   | 1:86:A:PHE:HD2  | 9        | 0.5           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2104) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HB  | 20       | 0.49          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 6        | 0.49          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 6        | 0.49          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 16       | 0.49          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 16       | 0.49          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 19       | 0.49          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 19       | 0.49          |
| (1,1978) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HD2 | 8        | 0.49          |
| (1,1978) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HD2 | 8        | 0.49          |
| (1,1978) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HD2 | 8        | 0.49          |
| (1,1687) | 1:142:A:TYR:HB3  | 1:142:A:TYR:HD2 | 7        | 0.49          |
| (1,1687) | 1:142:A:TYR:HB3  | 1:142:A:TYR:HD2 | 1        | 0.48          |
| (1,1687) | 1:142:A:TYR:HB3  | 1:142:A:TYR:HD2 | 20       | 0.48          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 18       | 0.48          |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 18       | 0.48          |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 18       | 0.48          |
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 18       | 0.48          |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 18       | 0.48          |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 18       | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 6        | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 6        | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 6        | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 6        | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 6        | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 6        | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 10       | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 10       | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 10       | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 10       | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 10       | 0.48          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 10       | 0.48          |
| (1,1677) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HD2 | 1        | 0.47          |
| (1,1677) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HD2 | 11       | 0.47          |
| (1,965)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HE1  | 1        | 0.47          |
| (1,965)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HE1  | 1        | 0.47          |
| (1,965)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HE1  | 1        | 0.47          |
| (1,1054) | 1:89:A:VAL:HG11  | 1:95:A:PHE:HD2  | 8        | 0.46          |
| (1,1054) | 1:89:A:VAL:HG12  | 1:95:A:PHE:HD2  | 8        | 0.46          |
| (1,1054) | 1:89:A:VAL:HG13  | 1:95:A:PHE:HD2  | 8        | 0.46          |
| (1,1054) | 1:89:A:VAL:HG21  | 1:95:A:PHE:HD2  | 8        | 0.46          |
| (1,1054) | 1:89:A:VAL:HG22  | 1:95:A:PHE:HD2  | 8        | 0.46          |
| (1,1054) | 1:89:A:VAL:HG23  | 1:95:A:PHE:HD2  | 8        | 0.46          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2104) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HB  | 16       | 0.45          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG2 | 2        | 0.45          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG3 | 2        | 0.45          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG2 | 20       | 0.45          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG3 | 20       | 0.45          |
| (1,1687) | 1:142:A:TYR:HB3 | 1:142:A:TYR:HD2 | 16       | 0.45          |
| (1,1675) | 1:141:A:PRO:HB2 | 1:142:A:TYR:HE2 | 7        | 0.45          |
| (1,973)  | 1:27:A:HIS:HD2  | 1:86:A:PHE:HD2  | 3        | 0.45          |
| (1,965)  | 1:24:A:VAL:HG21 | 1:86:A:PHE:HE1  | 16       | 0.45          |
| (1,965)  | 1:24:A:VAL:HG22 | 1:86:A:PHE:HE1  | 16       | 0.45          |
| (1,965)  | 1:24:A:VAL:HG23 | 1:86:A:PHE:HE1  | 16       | 0.45          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD11 | 7        | 0.45          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD12 | 7        | 0.45          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD13 | 7        | 0.45          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD21 | 7        | 0.45          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD22 | 7        | 0.45          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD23 | 7        | 0.45          |
| (1,2104) | 1:142:A:TYR:HD1 | 1:167:A:VAL:HB  | 11       | 0.44          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG2 | 12       | 0.44          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG3 | 12       | 0.44          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG2 | 13       | 0.44          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG3 | 13       | 0.44          |
| (1,1056) | 1:95:A:PHE:HA   | 1:95:A:PHE:HD2  | 9        | 0.44          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG2 | 15       | 0.43          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG3 | 15       | 0.43          |
| (1,967)  | 1:24:A:VAL:HG11 | 1:86:A:PHE:HD1  | 4        | 0.43          |
| (1,967)  | 1:24:A:VAL:HG12 | 1:86:A:PHE:HD1  | 4        | 0.43          |
| (1,967)  | 1:24:A:VAL:HG13 | 1:86:A:PHE:HD1  | 4        | 0.43          |
| (1,1055) | 1:94:A:SER:HA   | 1:95:A:PHE:HE2  | 18       | 0.42          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD11 | 11       | 0.42          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD12 | 11       | 0.42          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD13 | 11       | 0.42          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD21 | 11       | 0.42          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD22 | 11       | 0.42          |
| (1,897)  | 1:22:A:PHE:HE1  | 1:83:A:LEU:HD23 | 11       | 0.42          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG2 | 14       | 0.41          |
| (1,2011) | 1:161:A:PHE:HD2 | 1:163:A:MET:HG3 | 14       | 0.41          |
| (1,969)  | 1:24:A:VAL:HG11 | 1:86:A:PHE:HD1  | 18       | 0.41          |
| (1,969)  | 1:24:A:VAL:HG12 | 1:86:A:PHE:HD1  | 18       | 0.41          |
| (1,969)  | 1:24:A:VAL:HG13 | 1:86:A:PHE:HD1  | 18       | 0.41          |
| (1,969)  | 1:24:A:VAL:HG21 | 1:86:A:PHE:HD1  | 18       | 0.41          |
| (1,969)  | 1:24:A:VAL:HG22 | 1:86:A:PHE:HD1  | 18       | 0.41          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,969)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 18       | 0.41          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 5        | 0.41          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 5        | 0.41          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 5        | 0.41          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 5        | 0.41          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 5        | 0.41          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 5        | 0.41          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 8        | 0.4           |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 8        | 0.4           |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 8        | 0.4           |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 8        | 0.4           |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 8        | 0.4           |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 8        | 0.4           |
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 10       | 0.4           |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 13       | 0.4           |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 13       | 0.4           |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 13       | 0.4           |
| (1,2467) | 1:124:A:ALA:HA   | 1:189:A:PHE:HD1 | 17       | 0.39          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 4        | 0.39          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 4        | 0.39          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 7        | 0.39          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 7        | 0.39          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 18       | 0.39          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 18       | 0.39          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 9        | 0.39          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 9        | 0.39          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 9        | 0.39          |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 9        | 0.39          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 9        | 0.39          |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 9        | 0.39          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 10       | 0.38          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 10       | 0.38          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 6        | 0.38          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 6        | 0.38          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 6        | 0.38          |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 6        | 0.38          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 6        | 0.38          |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 6        | 0.38          |
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 19       | 0.38          |
| (1,969)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 19       | 0.38          |
| (1,969)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 19       | 0.38          |
| (1,969)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 19       | 0.38          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,969)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1  | 19       | 0.38          |
| (1,969)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1  | 19       | 0.38          |
| (1,969)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 19       | 0.38          |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 9        | 0.38          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 9        | 0.38          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 9        | 0.38          |
| (1,2104) | 1:142:A:TYR:HD1  | 1:167:A:VAL:HB  | 7        | 0.37          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 11       | 0.37          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 11       | 0.37          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 5        | 0.37          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 5        | 0.37          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 5        | 0.37          |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 5        | 0.37          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 5        | 0.37          |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 5        | 0.37          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 12       | 0.37          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 12       | 0.37          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 12       | 0.37          |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 12       | 0.37          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 12       | 0.37          |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 12       | 0.37          |
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 14       | 0.37          |
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 15       | 0.37          |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1  | 4        | 0.37          |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1  | 4        | 0.37          |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1  | 4        | 0.37          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 4        | 0.36          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 4        | 0.36          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 4        | 0.36          |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 4        | 0.36          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 4        | 0.36          |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 4        | 0.36          |
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 8        | 0.36          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 3        | 0.36          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 3        | 0.36          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 3        | 0.36          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 3        | 0.36          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 3        | 0.36          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 3        | 0.36          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 3        | 0.35          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 3        | 0.35          |
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 2        | 0.35          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 4        | 0.35          |
| (1,1056) | 1:95:A:PHE:HA    | 1:95:A:PHE:HD2  | 12       | 0.35          |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 3        | 0.35          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 3        | 0.35          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 3        | 0.35          |
| (1,2492) | 1:182:A:LYS:HE2  | 1:189:A:PHE:HE2 | 17       | 0.34          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD11 | 2        | 0.34          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD12 | 2        | 0.34          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD13 | 2        | 0.34          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD21 | 2        | 0.34          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD22 | 2        | 0.34          |
| (1,897)  | 1:22:A:PHE:HE1   | 1:83:A:LEU:HD23 | 2        | 0.34          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG2 | 9        | 0.33          |
| (1,2011) | 1:161:A:PHE:HD2  | 1:163:A:MET:HG3 | 9        | 0.33          |
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 2        | 0.33          |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 2        | 0.33          |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 2        | 0.33          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 2        | 0.33          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 2        | 0.33          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 2        | 0.33          |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 2        | 0.33          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 2        | 0.33          |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 2        | 0.33          |
| (1,969)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 20       | 0.33          |
| (1,969)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 20       | 0.33          |
| (1,969)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 20       | 0.33          |
| (1,969)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1  | 20       | 0.33          |
| (1,969)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1  | 20       | 0.33          |
| (1,969)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 20       | 0.33          |
| (1,1677) | 1:141:A:PRO:HB2  | 1:142:A:TYR:HD2 | 7        | 0.32          |
| (1,968)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1  | 18       | 0.32          |
| (1,968)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1  | 18       | 0.32          |
| (1,968)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 18       | 0.32          |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1  | 9        | 0.32          |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1  | 9        | 0.32          |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1  | 9        | 0.32          |
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 18       | 0.31          |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 18       | 0.31          |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 18       | 0.31          |
| (1,1649) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HE2 | 3        | 0.3           |
| (1,1649) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HE2 | 3        | 0.3           |
| (1,1649) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HE2 | 3        | 0.3           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1649) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HE2 | 3        | 0.3           |
| (1,1649) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HE2 | 3        | 0.3           |
| (1,1649) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HE2 | 3        | 0.3           |
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 16       | 0.29          |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 16       | 0.29          |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 16       | 0.29          |
| (1,969)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 8        | 0.29          |
| (1,969)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 8        | 0.29          |
| (1,969)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 8        | 0.29          |
| (1,969)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1  | 8        | 0.29          |
| (1,969)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1  | 8        | 0.29          |
| (1,969)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 8        | 0.29          |
| (1,968)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1  | 19       | 0.29          |
| (1,968)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1  | 19       | 0.29          |
| (1,968)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 19       | 0.29          |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1  | 13       | 0.29          |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1  | 13       | 0.29          |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1  | 13       | 0.29          |
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 6        | 0.28          |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 6        | 0.28          |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 6        | 0.28          |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 14       | 0.28          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 14       | 0.28          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 14       | 0.28          |
| (1,969)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 12       | 0.26          |
| (1,969)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 12       | 0.26          |
| (1,969)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 12       | 0.26          |
| (1,969)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1  | 12       | 0.26          |
| (1,969)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1  | 12       | 0.26          |
| (1,969)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 12       | 0.26          |
| (1,967)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 10       | 0.26          |
| (1,967)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 10       | 0.26          |
| (1,967)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 10       | 0.26          |
| (1,965)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HE1  | 13       | 0.26          |
| (1,965)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HE1  | 13       | 0.26          |
| (1,965)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HE1  | 13       | 0.26          |
| (1,965)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HE1  | 4        | 0.25          |
| (1,965)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HE1  | 4        | 0.25          |
| (1,965)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HE1  | 4        | 0.25          |
| (1,969)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 1        | 0.24          |
| (1,969)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 1        | 0.24          |
| (1,969)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 1        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,969)  | 1:24:A:VAL:HG21 | 1:86:A:PHE:HD1  | 1        | 0.24          |
| (1,969)  | 1:24:A:VAL:HG22 | 1:86:A:PHE:HD1  | 1        | 0.24          |
| (1,969)  | 1:24:A:VAL:HG23 | 1:86:A:PHE:HD1  | 1        | 0.24          |
| (1,967)  | 1:24:A:VAL:HG11 | 1:86:A:PHE:HD1  | 15       | 0.24          |
| (1,967)  | 1:24:A:VAL:HG12 | 1:86:A:PHE:HD1  | 15       | 0.24          |
| (1,967)  | 1:24:A:VAL:HG13 | 1:86:A:PHE:HD1  | 15       | 0.24          |
| (1,967)  | 1:24:A:VAL:HG11 | 1:86:A:PHE:HD1  | 6        | 0.23          |
| (1,967)  | 1:24:A:VAL:HG12 | 1:86:A:PHE:HD1  | 6        | 0.23          |
| (1,967)  | 1:24:A:VAL:HG13 | 1:86:A:PHE:HD1  | 6        | 0.23          |
| (1,967)  | 1:24:A:VAL:HG11 | 1:86:A:PHE:HD1  | 7        | 0.23          |
| (1,967)  | 1:24:A:VAL:HG12 | 1:86:A:PHE:HD1  | 7        | 0.23          |
| (1,967)  | 1:24:A:VAL:HG13 | 1:86:A:PHE:HD1  | 7        | 0.23          |
| (1,1977) | 1:152:A:ALA:HB1 | 1:161:A:PHE:HE2 | 19       | 0.22          |
| (1,1977) | 1:152:A:ALA:HB2 | 1:161:A:PHE:HE2 | 19       | 0.22          |
| (1,1977) | 1:152:A:ALA:HB3 | 1:161:A:PHE:HE2 | 19       | 0.22          |
| (1,968)  | 1:24:A:VAL:HG21 | 1:86:A:PHE:HD1  | 20       | 0.22          |
| (1,968)  | 1:24:A:VAL:HG22 | 1:86:A:PHE:HD1  | 20       | 0.22          |
| (1,968)  | 1:24:A:VAL:HG23 | 1:86:A:PHE:HD1  | 20       | 0.22          |
| (1,967)  | 1:24:A:VAL:HG11 | 1:86:A:PHE:HD1  | 2        | 0.22          |
| (1,967)  | 1:24:A:VAL:HG12 | 1:86:A:PHE:HD1  | 2        | 0.22          |
| (1,967)  | 1:24:A:VAL:HG13 | 1:86:A:PHE:HD1  | 2        | 0.22          |
| (1,967)  | 1:24:A:VAL:HG11 | 1:86:A:PHE:HD1  | 5        | 0.22          |
| (1,967)  | 1:24:A:VAL:HG12 | 1:86:A:PHE:HD1  | 5        | 0.22          |
| (1,967)  | 1:24:A:VAL:HG13 | 1:86:A:PHE:HD1  | 5        | 0.22          |
| (1,967)  | 1:24:A:VAL:HG11 | 1:86:A:PHE:HD1  | 11       | 0.22          |
| (1,967)  | 1:24:A:VAL:HG12 | 1:86:A:PHE:HD1  | 11       | 0.22          |
| (1,967)  | 1:24:A:VAL:HG13 | 1:86:A:PHE:HD1  | 11       | 0.22          |
| (1,1977) | 1:152:A:ALA:HB1 | 1:161:A:PHE:HE2 | 4        | 0.2           |
| (1,1977) | 1:152:A:ALA:HB2 | 1:161:A:PHE:HE2 | 4        | 0.2           |
| (1,1977) | 1:152:A:ALA:HB3 | 1:161:A:PHE:HE2 | 4        | 0.2           |
| (1,1977) | 1:152:A:ALA:HB1 | 1:161:A:PHE:HE2 | 5        | 0.2           |
| (1,1977) | 1:152:A:ALA:HB2 | 1:161:A:PHE:HE2 | 5        | 0.2           |
| (1,1977) | 1:152:A:ALA:HB3 | 1:161:A:PHE:HE2 | 5        | 0.2           |
| (1,965)  | 1:24:A:VAL:HG21 | 1:86:A:PHE:HE1  | 9        | 0.2           |
| (1,965)  | 1:24:A:VAL:HG22 | 1:86:A:PHE:HE1  | 9        | 0.2           |
| (1,965)  | 1:24:A:VAL:HG23 | 1:86:A:PHE:HE1  | 9        | 0.2           |
| (1,1977) | 1:152:A:ALA:HB1 | 1:161:A:PHE:HE2 | 11       | 0.19          |
| (1,1977) | 1:152:A:ALA:HB2 | 1:161:A:PHE:HE2 | 11       | 0.19          |
| (1,1977) | 1:152:A:ALA:HB3 | 1:161:A:PHE:HE2 | 11       | 0.19          |
| (1,1977) | 1:152:A:ALA:HB1 | 1:161:A:PHE:HE2 | 13       | 0.19          |
| (1,1977) | 1:152:A:ALA:HB2 | 1:161:A:PHE:HE2 | 13       | 0.19          |
| (1,1977) | 1:152:A:ALA:HB3 | 1:161:A:PHE:HE2 | 13       | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 17       | 0.19          |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 17       | 0.19          |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 17       | 0.19          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 17       | 0.19          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 17       | 0.19          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 17       | 0.19          |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 17       | 0.19          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 17       | 0.19          |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 17       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 16       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 16       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 16       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1  | 16       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1  | 16       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 16       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HD1  | 17       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HD1  | 17       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HD1  | 17       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1  | 17       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1  | 17       | 0.19          |
| (1,969)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 17       | 0.19          |
| (1,2501) | 1:182:A:LYS:HD3  | 1:189:A:PHE:HE2 | 17       | 0.18          |
| (1,968)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1  | 8        | 0.18          |
| (1,968)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1  | 8        | 0.18          |
| (1,968)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 8        | 0.18          |
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 3        | 0.17          |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 3        | 0.17          |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 3        | 0.17          |
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 1        | 0.16          |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 1        | 0.16          |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 1        | 0.16          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 11       | 0.16          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 11       | 0.16          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 11       | 0.16          |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 11       | 0.16          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 11       | 0.16          |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 11       | 0.16          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 14       | 0.16          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 14       | 0.16          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 14       | 0.16          |
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 14       | 0.16          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 14       | 0.16          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 14       | 0.16          |
| (1,966)  | 1:24:A:VAL:HG11  | 1:86:A:PHE:HE1  | 3        | 0.16          |
| (1,966)  | 1:24:A:VAL:HG12  | 1:86:A:PHE:HE1  | 3        | 0.16          |
| (1,966)  | 1:24:A:VAL:HG13  | 1:86:A:PHE:HE1  | 3        | 0.16          |
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 14       | 0.15          |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 14       | 0.15          |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 14       | 0.15          |
| (1,973)  | 1:27:A:HIS:HD2   | 1:86:A:PHE:HD2  | 19       | 0.15          |
| (1,968)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1  | 12       | 0.15          |
| (1,968)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1  | 12       | 0.15          |
| (1,968)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 12       | 0.15          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 4        | 0.15          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 16       | 0.15          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 17       | 0.15          |
| (1,973)  | 1:27:A:HIS:HD2   | 1:86:A:PHE:HD2  | 12       | 0.14          |
| (1,973)  | 1:27:A:HIS:HD2   | 1:86:A:PHE:HD2  | 20       | 0.14          |
| (1,811)  | 1:71:A:LYS:HA    | 1:71:A:LYS:HG2  | 2        | 0.14          |
| (1,811)  | 1:71:A:LYS:HA    | 1:71:A:LYS:HG3  | 2        | 0.14          |
| (1,811)  | 1:71:A:LYS:HA    | 1:71:A:LYS:HG2  | 4        | 0.14          |
| (1,811)  | 1:71:A:LYS:HA    | 1:71:A:LYS:HG3  | 4        | 0.14          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 1        | 0.14          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 8        | 0.14          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 9        | 0.14          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 10       | 0.14          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 12       | 0.14          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 20       | 0.14          |
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 15       | 0.13          |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 15       | 0.13          |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 15       | 0.13          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 7        | 0.13          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 11       | 0.13          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 13       | 0.13          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 18       | 0.13          |
| (1,741)  | 1:65:A:LYS:HB3   | 1:66:A:LYS:H    | 19       | 0.13          |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB2  | 17       | 0.13          |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB3  | 17       | 0.13          |
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 9        | 0.12          |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 9        | 0.12          |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 9        | 0.12          |
| (1,1650) | 1:139:A:LEU:HD11 | 1:140:A:PHE:HD2 | 15       | 0.12          |
| (1,1650) | 1:139:A:LEU:HD12 | 1:140:A:PHE:HD2 | 15       | 0.12          |
| (1,1650) | 1:139:A:LEU:HD13 | 1:140:A:PHE:HD2 | 15       | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1650) | 1:139:A:LEU:HD21 | 1:140:A:PHE:HD2 | 15       | 0.12          |
| (1,1650) | 1:139:A:LEU:HD22 | 1:140:A:PHE:HD2 | 15       | 0.12          |
| (1,1650) | 1:139:A:LEU:HD23 | 1:140:A:PHE:HD2 | 15       | 0.12          |
| (1,968)  | 1:24:A:VAL:HG21  | 1:86:A:PHE:HD1  | 1        | 0.12          |
| (1,968)  | 1:24:A:VAL:HG22  | 1:86:A:PHE:HD1  | 1        | 0.12          |
| (1,968)  | 1:24:A:VAL:HG23  | 1:86:A:PHE:HD1  | 1        | 0.12          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 8        | 0.12          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 9        | 0.12          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 10       | 0.12          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 11       | 0.12          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 12       | 0.12          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 13       | 0.12          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 17       | 0.12          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 20       | 0.12          |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB2  | 1        | 0.12          |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB3  | 1        | 0.12          |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB2  | 4        | 0.12          |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB3  | 4        | 0.12          |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB2  | 8        | 0.12          |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB3  | 8        | 0.12          |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB2  | 16       | 0.12          |
| (1,736)  | 1:65:A:LYS:H     | 1:65:A:LYS:HB3  | 16       | 0.12          |
| (1,1977) | 1:152:A:ALA:HB1  | 1:161:A:PHE:HE2 | 10       | 0.11          |
| (1,1977) | 1:152:A:ALA:HB2  | 1:161:A:PHE:HE2 | 10       | 0.11          |
| (1,1977) | 1:152:A:ALA:HB3  | 1:161:A:PHE:HE2 | 10       | 0.11          |
| (1,1054) | 1:89:A:VAL:HG11  | 1:95:A:PHE:HD2  | 14       | 0.11          |
| (1,1054) | 1:89:A:VAL:HG12  | 1:95:A:PHE:HD2  | 14       | 0.11          |
| (1,1054) | 1:89:A:VAL:HG13  | 1:95:A:PHE:HD2  | 14       | 0.11          |
| (1,1054) | 1:89:A:VAL:HG21  | 1:95:A:PHE:HD2  | 14       | 0.11          |
| (1,1054) | 1:89:A:VAL:HG22  | 1:95:A:PHE:HD2  | 14       | 0.11          |
| (1,1054) | 1:89:A:VAL:HG23  | 1:95:A:PHE:HD2  | 14       | 0.11          |
| (1,973)  | 1:27:A:HIS:HD2   | 1:86:A:PHE:HD2  | 17       | 0.11          |
| (1,811)  | 1:71:A:LYS:HA    | 1:71:A:LYS:HG2  | 5        | 0.11          |
| (1,811)  | 1:71:A:LYS:HA    | 1:71:A:LYS:HG3  | 5        | 0.11          |
| (1,811)  | 1:71:A:LYS:HA    | 1:71:A:LYS:HG2  | 15       | 0.11          |
| (1,811)  | 1:71:A:LYS:HA    | 1:71:A:LYS:HG3  | 15       | 0.11          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 1        | 0.11          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 4        | 0.11          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 7        | 0.11          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 16       | 0.11          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 18       | 0.11          |
| (1,739)  | 1:65:A:LYS:H     | 1:66:A:LYS:HA   | 19       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB2  | 7        | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB3  | 7        | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB2  | 9        | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB3  | 9        | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB2  | 10       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB3  | 10       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB2  | 11       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB3  | 11       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB2  | 12       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB3  | 12       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB2  | 13       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB3  | 13       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB2  | 18       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB3  | 18       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB2  | 19       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB3  | 19       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB2  | 20       | 0.11          |
| (1,736)  | 1:65:A:LYS:H    | 1:65:A:LYS:HB3  | 20       | 0.11          |
| (1,663)  | 1:36:A:GLU:HG2  | 1:60:A:LEU:HG   | 14       | 0.11          |
| (1,663)  | 1:36:A:GLU:HG3  | 1:60:A:LEU:HG   | 14       | 0.11          |
| (1,663)  | 1:36:A:GLU:HG2  | 1:60:A:LEU:HG   | 15       | 0.11          |
| (1,663)  | 1:36:A:GLU:HG3  | 1:60:A:LEU:HG   | 15       | 0.11          |
| (1,663)  | 1:36:A:GLU:HG2  | 1:60:A:LEU:HG   | 18       | 0.11          |
| (1,663)  | 1:36:A:GLU:HG3  | 1:60:A:LEU:HG   | 18       | 0.11          |
| (1,663)  | 1:36:A:GLU:HG2  | 1:60:A:LEU:HG   | 19       | 0.11          |
| (1,663)  | 1:36:A:GLU:HG3  | 1:60:A:LEU:HG   | 19       | 0.11          |
| (1,47)   | 1:14:A:PRO:HB2  | 1:15:A:ASP:H    | 20       | 0.11          |
| (1,47)   | 1:14:A:PRO:HB3  | 1:15:A:ASP:H    | 20       | 0.11          |
| (1,1977) | 1:152:A:ALA:HB1 | 1:161:A:PHE:HE2 | 12       | 0.1           |
| (1,1977) | 1:152:A:ALA:HB2 | 1:161:A:PHE:HE2 | 12       | 0.1           |
| (1,1977) | 1:152:A:ALA:HB3 | 1:161:A:PHE:HE2 | 12       | 0.1           |
| (1,965)  | 1:24:A:VAL:HG21 | 1:86:A:PHE:HE1  | 3        | 0.1           |
| (1,965)  | 1:24:A:VAL:HG22 | 1:86:A:PHE:HE1  | 3        | 0.1           |
| (1,965)  | 1:24:A:VAL:HG23 | 1:86:A:PHE:HE1  | 3        | 0.1           |
| (1,811)  | 1:71:A:LYS:HA   | 1:71:A:LYS:HG2  | 9        | 0.1           |
| (1,811)  | 1:71:A:LYS:HA   | 1:71:A:LYS:HG3  | 9        | 0.1           |
| (1,811)  | 1:71:A:LYS:HA   | 1:71:A:LYS:HG2  | 10       | 0.1           |
| (1,811)  | 1:71:A:LYS:HA   | 1:71:A:LYS:HG3  | 10       | 0.1           |
| (1,811)  | 1:71:A:LYS:HA   | 1:71:A:LYS:HG2  | 17       | 0.1           |
| (1,811)  | 1:71:A:LYS:HA   | 1:71:A:LYS:HG3  | 17       | 0.1           |
| (1,663)  | 1:36:A:GLU:HG2  | 1:60:A:LEU:HG   | 5        | 0.1           |
| (1,663)  | 1:36:A:GLU:HG3  | 1:60:A:LEU:HG   | 5        | 0.1           |

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| Key     | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|---------|----------------|---------------|----------|---------------|
| (1,663) | 1:36:A:GLU:HG2 | 1:60:A:LEU:HG | 6        | 0.1           |
| (1,663) | 1:36:A:GLU:HG3 | 1:60:A:LEU:HG | 6        | 0.1           |
| (1,663) | 1:36:A:GLU:HG2 | 1:60:A:LEU:HG | 7        | 0.1           |
| (1,663) | 1:36:A:GLU:HG3 | 1:60:A:LEU:HG | 7        | 0.1           |
| (1,663) | 1:36:A:GLU:HG2 | 1:60:A:LEU:HG | 9        | 0.1           |
| (1,663) | 1:36:A:GLU:HG3 | 1:60:A:LEU:HG | 9        | 0.1           |
| (1,663) | 1:36:A:GLU:HG2 | 1:60:A:LEU:HG | 11       | 0.1           |
| (1,663) | 1:36:A:GLU:HG3 | 1:60:A:LEU:HG | 11       | 0.1           |
| (1,663) | 1:36:A:GLU:HG2 | 1:60:A:LEU:HG | 13       | 0.1           |
| (1,663) | 1:36:A:GLU:HG3 | 1:60:A:LEU:HG | 13       | 0.1           |
| (1,663) | 1:36:A:GLU:HG2 | 1:60:A:LEU:HG | 20       | 0.1           |
| (1,663) | 1:36:A:GLU:HG3 | 1:60:A:LEU:HG | 20       | 0.1           |
| (1,47)  | 1:14:A:PRO:HB2 | 1:15:A:ASP:H  | 8        | 0.1           |
| (1,47)  | 1:14:A:PRO:HB3 | 1:15:A:ASP:H  | 8        | 0.1           |

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

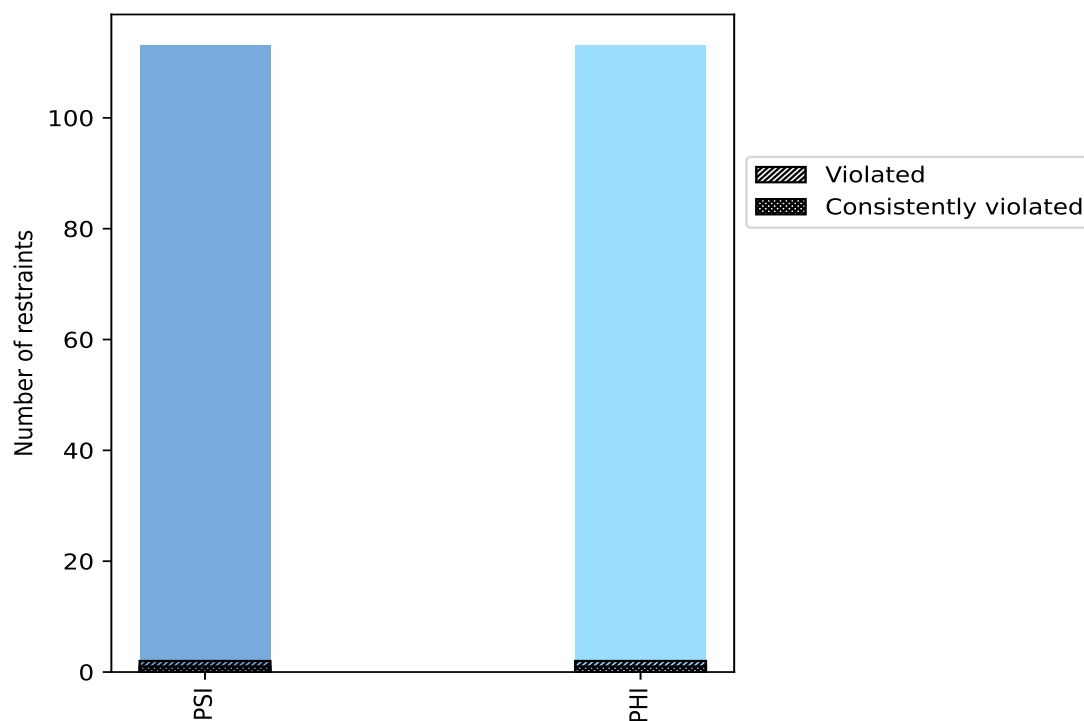
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 113   | 50.0           | 2                     | 1.8            | 0.9            | 1                                  | 0.9            | 0.4            |
| PHI        | 113   | 50.0           | 2                     | 1.8            | 0.9            | 1                                  | 0.9            | 0.4            |
| Total      | 226   | 100.0          | 4                     | 1.8            | 1.8            | 2                                  | 0.9            | 0.9            |

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

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



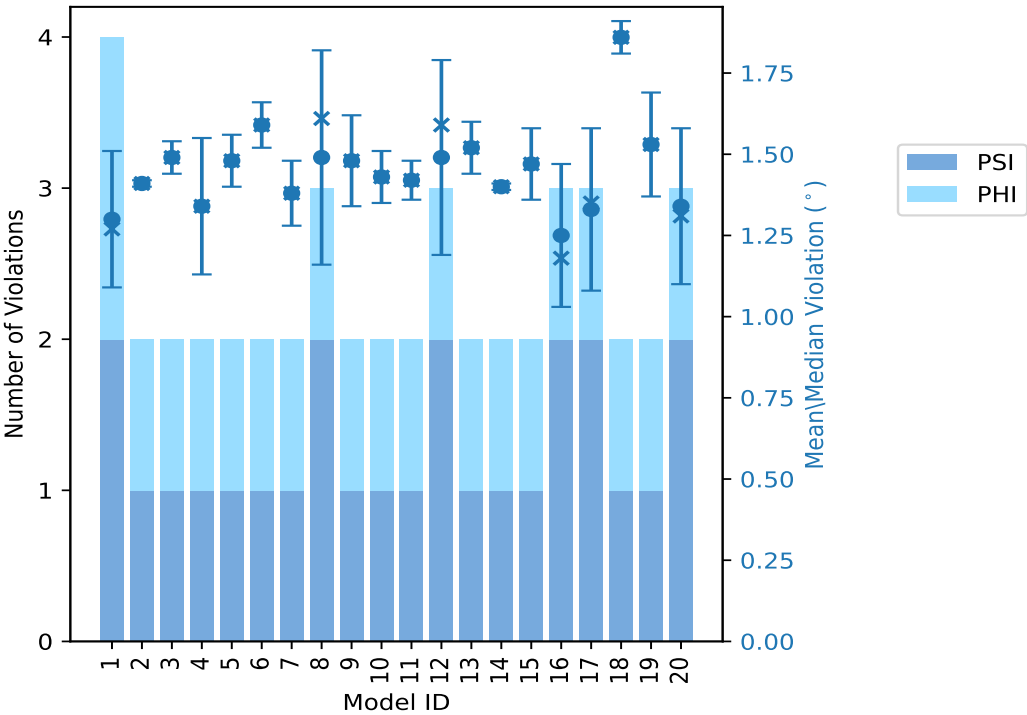
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 2                    | 2   | 4     | 1.3      | 1.57    | 0.21   | 1.27       |
| 2        | 1                    | 1   | 2     | 1.41     | 1.42    | 0.01   | 1.41       |
| 3        | 1                    | 1   | 2     | 1.49     | 1.54    | 0.05   | 1.49       |
| 4        | 1                    | 1   | 2     | 1.34     | 1.55    | 0.21   | 1.34       |
| 5        | 1                    | 1   | 2     | 1.48     | 1.55    | 0.08   | 1.48       |
| 6        | 1                    | 1   | 2     | 1.59     | 1.66    | 0.07   | 1.59       |
| 7        | 1                    | 1   | 2     | 1.38     | 1.48    | 0.1    | 1.38       |
| 8        | 2                    | 1   | 3     | 1.49     | 1.82    | 0.33   | 1.61       |
| 9        | 1                    | 1   | 2     | 1.48     | 1.63    | 0.14   | 1.48       |
| 10       | 1                    | 1   | 2     | 1.43     | 1.51    | 0.08   | 1.43       |
| 11       | 1                    | 1   | 2     | 1.42     | 1.48    | 0.06   | 1.42       |
| 12       | 2                    | 1   | 3     | 1.49     | 1.8     | 0.3    | 1.59       |
| 13       | 1                    | 1   | 2     | 1.52     | 1.6     | 0.08   | 1.52       |
| 14       | 1                    | 1   | 2     | 1.4      | 1.41    | 0.01   | 1.4        |
| 15       | 1                    | 1   | 2     | 1.47     | 1.58    | 0.11   | 1.47       |
| 16       | 2                    | 1   | 3     | 1.25     | 1.55    | 0.22   | 1.18       |
| 17       | 2                    | 1   | 3     | 1.33     | 1.62    | 0.25   | 1.35       |
| 18       | 1                    | 1   | 2     | 1.86     | 1.91    | 0.05   | 1.86       |
| 19       | 1                    | 1   | 2     | 1.53     | 1.69    | 0.16   | 1.53       |
| 20       | 2                    | 1   | 3     | 1.34     | 1.65    | 0.24   | 1.31       |

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



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

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

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

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

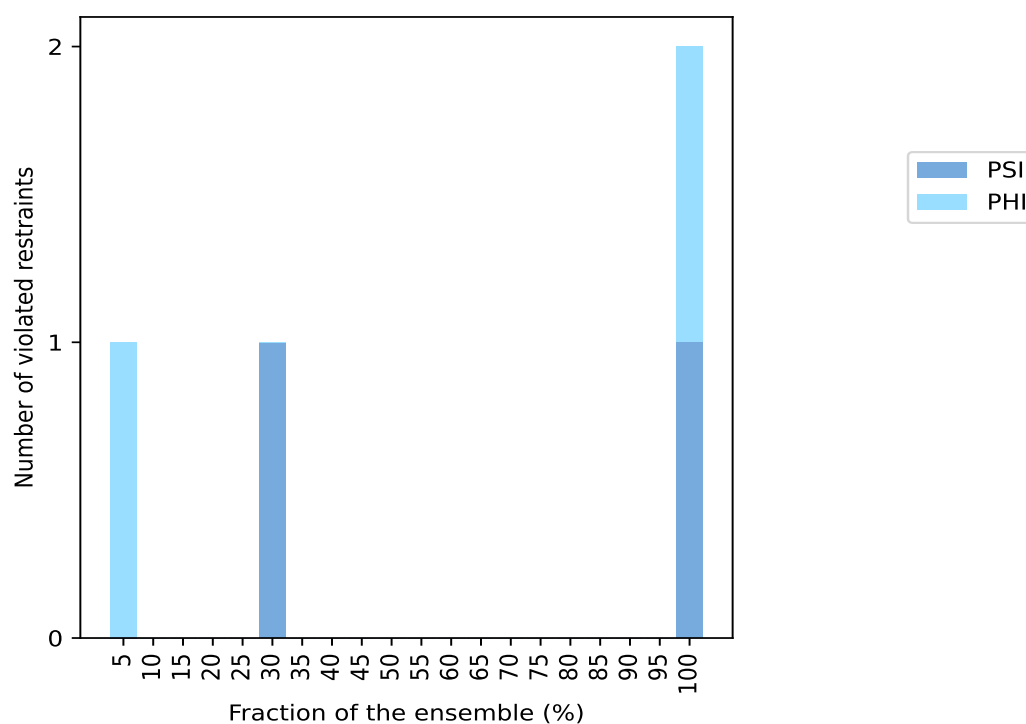
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |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

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

### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)

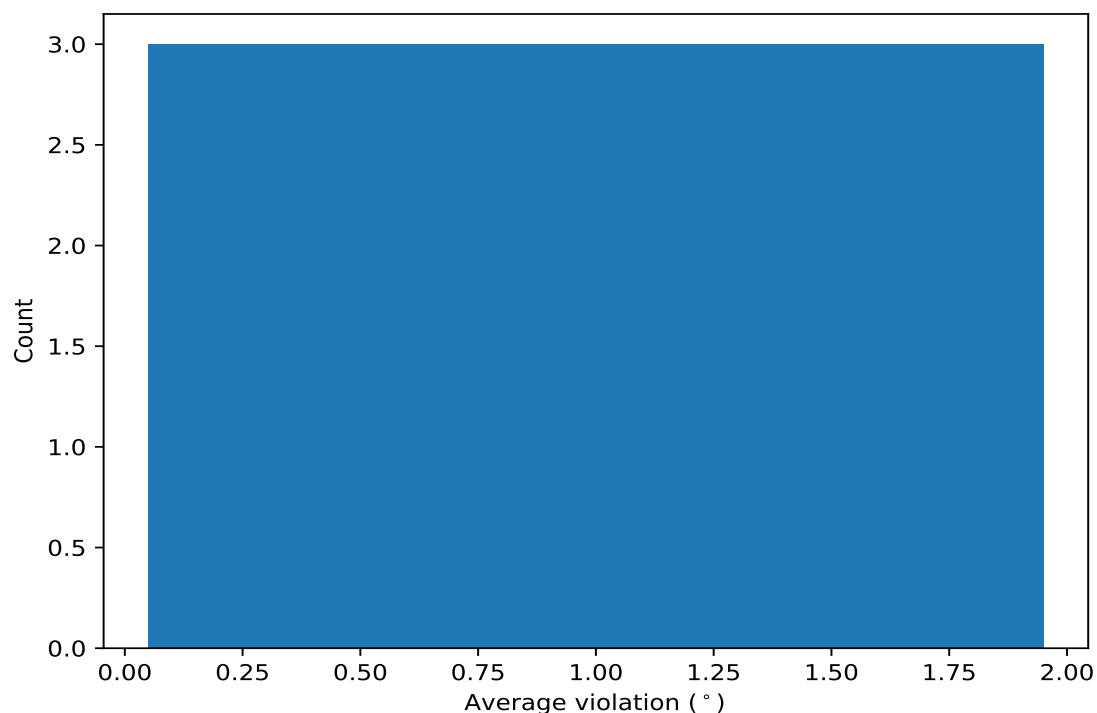


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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

in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle 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.

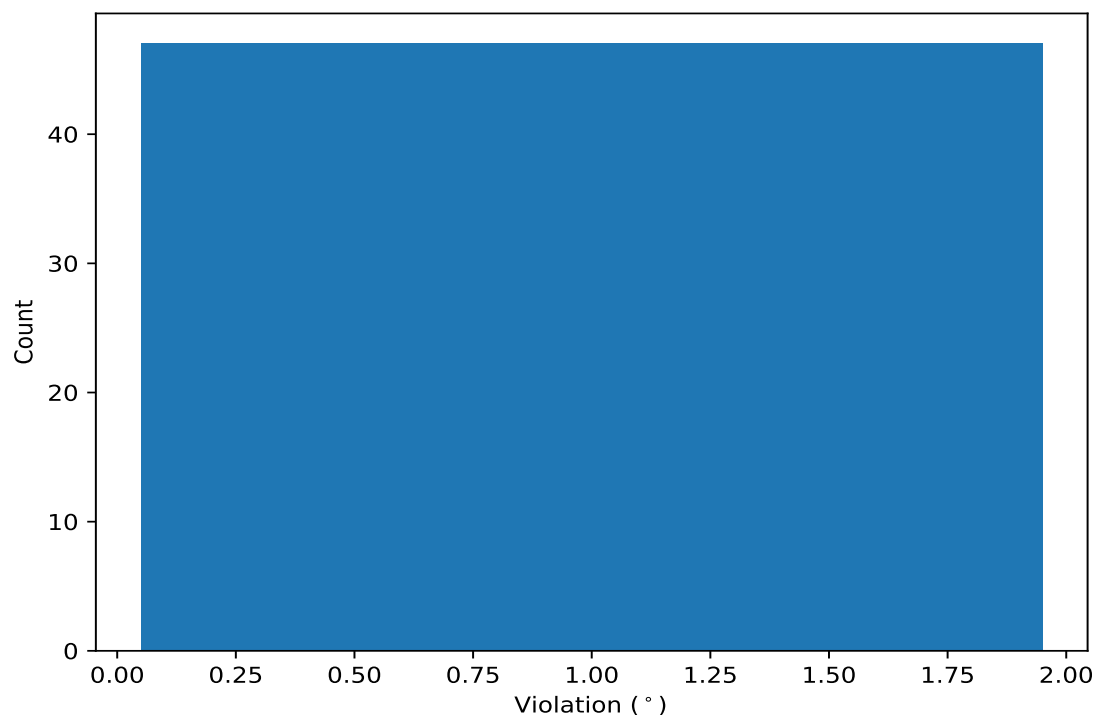
| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 20                  | 1.6  | 0.13            | 1.58   |
| (1,33) | 1:30:A:LYS:C | 1:31:A:GLU:N  | 1:31:A:GLU:CA | 1:31:A:GLU:C | 20                  | 1.39 | 0.16            | 1.37   |
| (1,34) | 1:31:A:GLU:N | 1:31:A:GLU:CA | 1:31:A:GLU:C  | 1:32:A:ASN:N | 6                   | 1.06 | 0.03            | 1.05   |

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

### 10.5 All violated dihedral-angle restraints [i](#)

#### 10.5.1 Histogram : Distribution of violations [i](#)

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



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

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

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 18       | 1.91          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 8        | 1.82          |
| (1,33) | 1:30:A:LYS:C | 1:31:A:GLU:N  | 1:31:A:GLU:CA | 1:31:A:GLU:C | 18       | 1.81          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 12       | 1.8           |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 19       | 1.69          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 6        | 1.66          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 20       | 1.65          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 9        | 1.63          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 17       | 1.62          |
| (1,33) | 1:30:A:LYS:C | 1:31:A:GLU:N  | 1:31:A:GLU:CA | 1:31:A:GLU:C | 8        | 1.61          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 13       | 1.6           |
| (1,33) | 1:30:A:LYS:C | 1:31:A:GLU:N  | 1:31:A:GLU:CA | 1:31:A:GLU:C | 12       | 1.59          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 15       | 1.58          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 1        | 1.57          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 4        | 1.55          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 5        | 1.55          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 16       | 1.55          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 3        | 1.54          |
| (1,33) | 1:30:A:LYS:C | 1:31:A:GLU:N  | 1:31:A:GLU:CA | 1:31:A:GLU:C | 6        | 1.52          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 10       | 1.51          |
| (1,32) | 1:30:A:LYS:N | 1:30:A:LYS:CA | 1:30:A:LYS:C  | 1:31:A:GLU:N | 7        | 1.48          |

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| Key     | Atom-1        | Atom-2        | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|---------------|----------------|---------------|----------|---------------|
| (1,32)  | 1:30:A:LYS:N  | 1:30:A:LYS:CA | 1:30:A:LYS:C   | 1:31:A:GLU:N  | 11       | 1.48          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 3        | 1.44          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 13       | 1.44          |
| (1,143) | 1:134:A:GLU:C | 1:135:A:ARG:N | 1:135:A:ARG:CA | 1:135:A:ARG:C | 1        | 1.43          |
| (1,32)  | 1:30:A:LYS:N  | 1:30:A:LYS:CA | 1:30:A:LYS:C   | 1:31:A:GLU:N  | 2        | 1.42          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 14       | 1.41          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 2        | 1.4           |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 5        | 1.4           |
| (1,32)  | 1:30:A:LYS:N  | 1:30:A:LYS:CA | 1:30:A:LYS:C   | 1:31:A:GLU:N  | 14       | 1.4           |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 19       | 1.37          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 15       | 1.36          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 10       | 1.35          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 11       | 1.35          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 17       | 1.35          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 9        | 1.34          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 20       | 1.31          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 7        | 1.28          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 16       | 1.18          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 4        | 1.13          |
| (1,34)  | 1:31:A:GLU:N  | 1:31:A:GLU:CA | 1:31:A:GLU:C   | 1:32:A:ASN:N  | 1        | 1.11          |
| (1,34)  | 1:31:A:GLU:N  | 1:31:A:GLU:CA | 1:31:A:GLU:C   | 1:32:A:ASN:N  | 12       | 1.09          |
| (1,33)  | 1:30:A:LYS:C  | 1:31:A:GLU:N  | 1:31:A:GLU:CA  | 1:31:A:GLU:C  | 1        | 1.07          |
| (1,34)  | 1:31:A:GLU:N  | 1:31:A:GLU:CA | 1:31:A:GLU:C   | 1:32:A:ASN:N  | 20       | 1.06          |
| (1,34)  | 1:31:A:GLU:N  | 1:31:A:GLU:CA | 1:31:A:GLU:C   | 1:32:A:ASN:N  | 8        | 1.04          |
| (1,34)  | 1:31:A:GLU:N  | 1:31:A:GLU:CA | 1:31:A:GLU:C   | 1:32:A:ASN:N  | 16       | 1.02          |
| (1,34)  | 1:31:A:GLU:N  | 1:31:A:GLU:CA | 1:31:A:GLU:C   | 1:32:A:ASN:N  | 17       | 1.02          |