



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 3, 2023 – 08:59 PM EDT

PDB ID : 2K49  
BMRB ID : 15791  
Title : Solution NMR structure of UPF0339 protein SO3888 from *Shewanella oneidensis*. Northeast Structural Genomics Consortium target SoR190  
Authors : Tang, Y.; Wang, D.; Nwosu, C.; Maglaqui, M.; Xiao, R.; Liu, J.; Baran, M.C.; Swapna, G.V.T.; Acton, T.B.; Rost, B.; Montelione, G.T.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2008-05-31

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)

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<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 : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

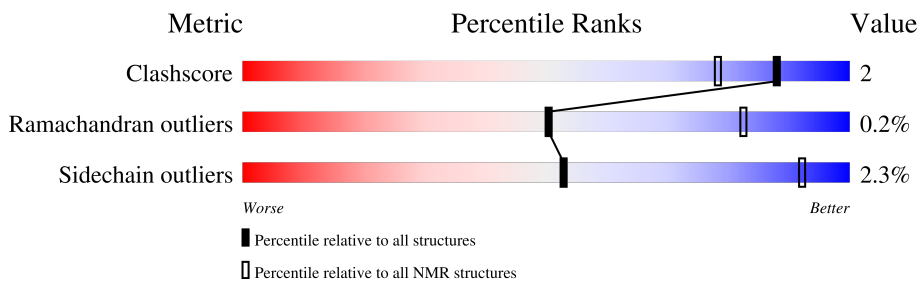
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 93%.

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            | 158937                      | 12864                     |
| Ramachandran outliers | 154571                      | 11451                     |
| Sidechain outliers    | 154315                      | 11428                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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     | 118    | <br>92% 8%       |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:3-A:111 (109)       | 0.78              | 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 3 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1823 atoms, of which 903 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UPF0339 protein SO\_3888.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
|     |       |          | Total | C   | H   | N   | O   | S |       |
| 1   | A     | 118      | 1823  | 571 | 903 | 163 | 182 | 4 | 0     |

There are 8 discrepancies between the modelled and reference sequences:

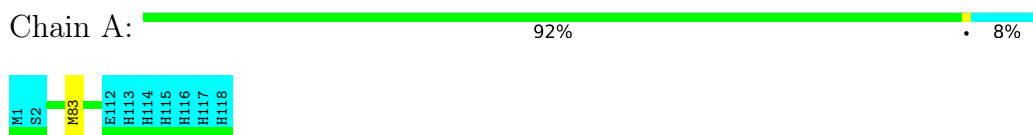
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 111     | LEU      | -      | expression tag | UNP Q8EAL4 |
| A     | 112     | GLU      | -      | expression tag | UNP Q8EAL4 |
| A     | 113     | HIS      | -      | expression tag | UNP Q8EAL4 |
| A     | 114     | HIS      | -      | expression tag | UNP Q8EAL4 |
| A     | 115     | HIS      | -      | expression tag | UNP Q8EAL4 |
| A     | 116     | HIS      | -      | expression tag | UNP Q8EAL4 |
| A     | 117     | HIS      | -      | expression tag | UNP Q8EAL4 |
| A     | 118     | HIS      | -      | expression tag | UNP Q8EAL4 |

## 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: UPF0339 protein SO\_3888

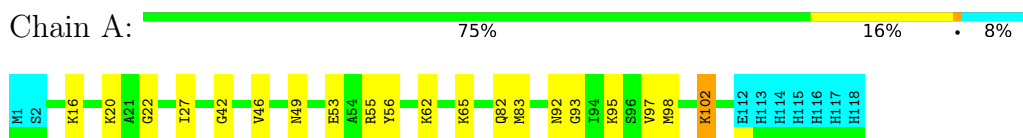


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

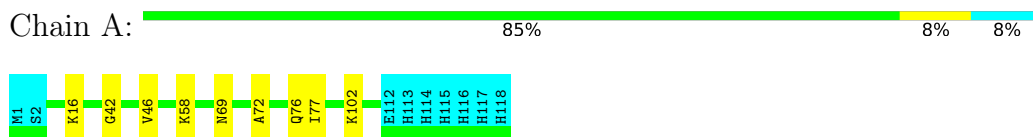
#### 4.2.1 Score per residue for model 1

- Molecule 1: UPF0339 protein SO\_3888



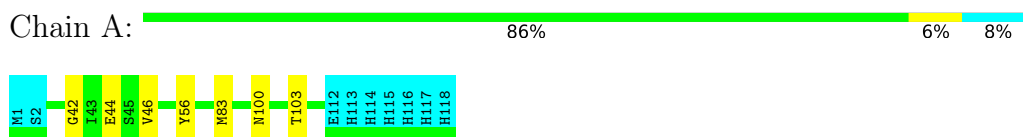
#### 4.2.2 Score per residue for model 2

- Molecule 1: UPF0339 protein SO\_3888



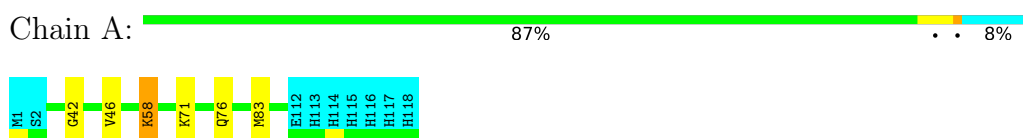
### 4.2.3 Score per residue for model 3

- Molecule 1: UPF0339 protein SO\_3888



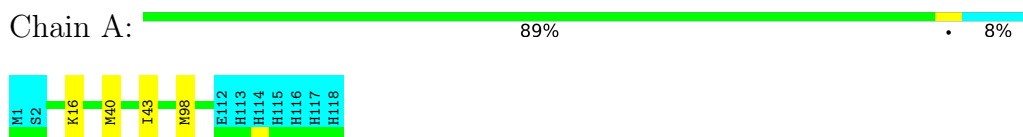
### 4.2.4 Score per residue for model 4

- Molecule 1: UPF0339 protein SO\_3888



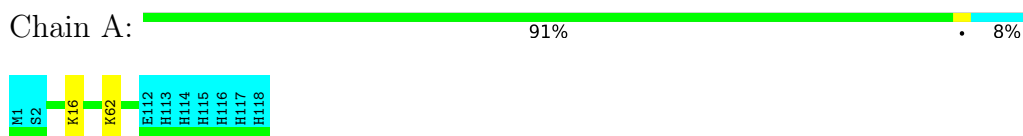
### 4.2.5 Score per residue for model 5

- Molecule 1: UPF0339 protein SO\_3888



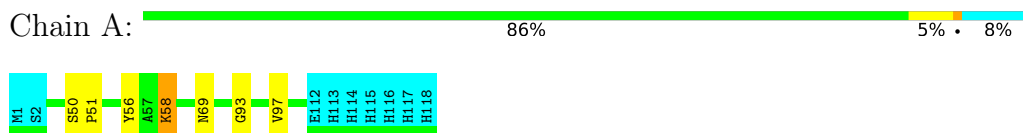
### 4.2.6 Score per residue for model 6

- Molecule 1: UPF0339 protein SO\_3888



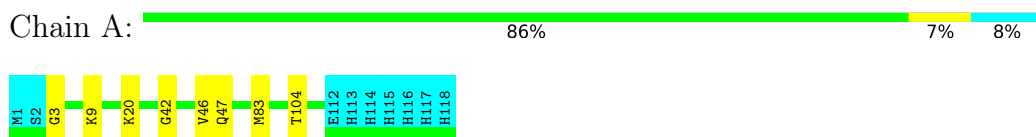
### 4.2.7 Score per residue for model 7

- Molecule 1: UPF0339 protein SO\_3888



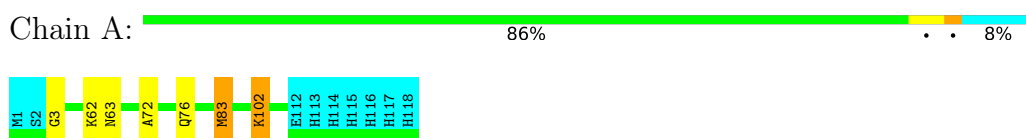
#### 4.2.8 Score per residue for model 8

- Molecule 1: UPF0339 protein SO\_3888



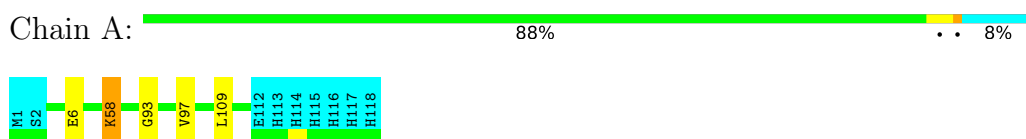
#### 4.2.9 Score per residue for model 9

- Molecule 1: UPF0339 protein SO\_3888



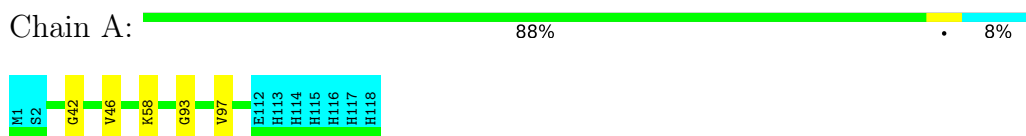
#### 4.2.10 Score per residue for model 10

- Molecule 1: UPF0339 protein SO\_3888



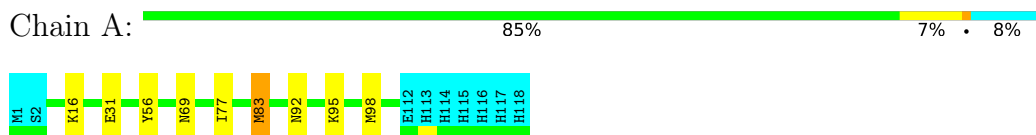
#### 4.2.11 Score per residue for model 11

- Molecule 1: UPF0339 protein SO\_3888



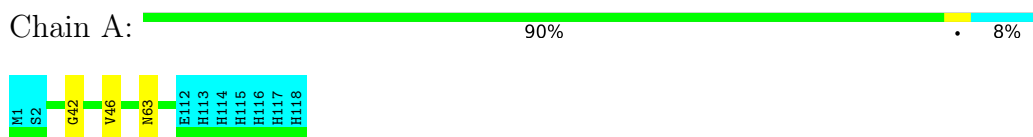
#### 4.2.12 Score per residue for model 12

- Molecule 1: UPF0339 protein SO\_3888



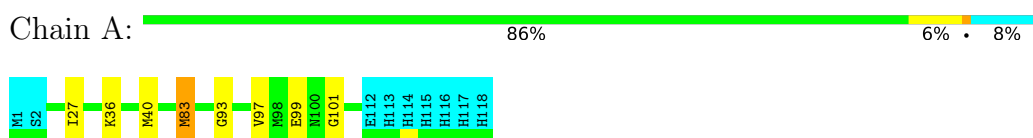
#### 4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: UPF0339 protein SO\_3888



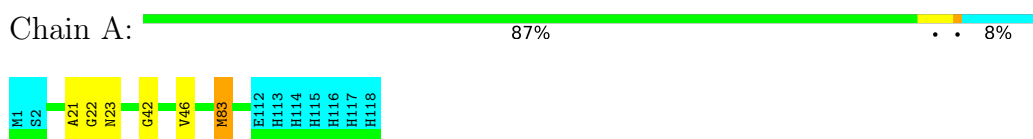
#### 4.2.14 Score per residue for model 14

- Molecule 1: UPF0339 protein SO\_3888



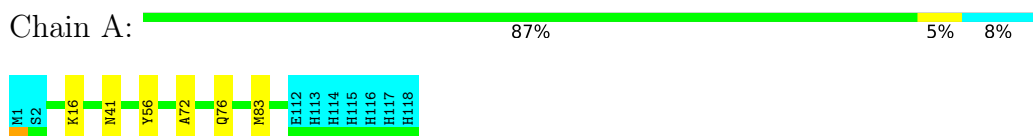
#### 4.2.15 Score per residue for model 15

- Molecule 1: UPF0339 protein SO\_3888



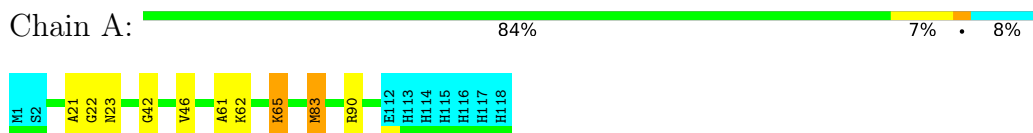
#### 4.2.16 Score per residue for model 16

- Molecule 1: UPF0339 protein SO\_3888



#### 4.2.17 Score per residue for model 17

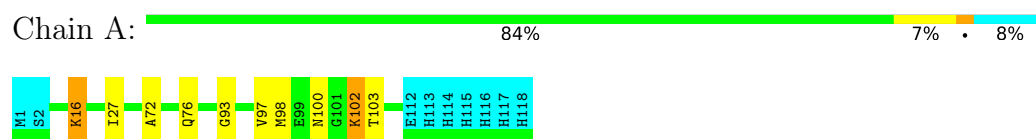
- Molecule 1: UPF0339 protein SO\_3888





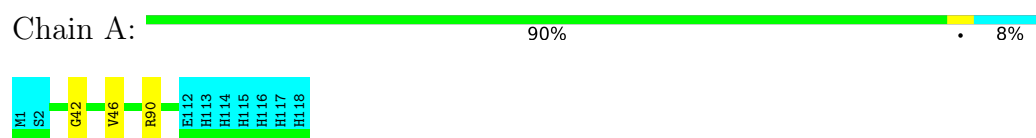
#### 4.2.18 Score per residue for model 18

- Molecule 1: UPF0339 protein SO\_3888



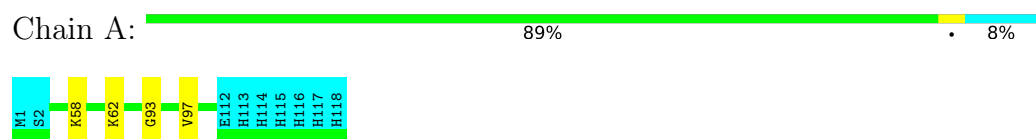
#### 4.2.19 Score per residue for model 19

- Molecule 1: UPF0339 protein SO\_3888



#### 4.2.20 Score per residue for model 20

- Molecule 1: UPF0339 protein SO\_3888



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| AutoStructure | structure solution | 2.2.1   |
| CYANA         | structure solution | 2.1     |
| CNS           | refinement         | 1.1     |

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                       | 1353           |
| Number of shifts mapped to atoms             | 1353           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 93%            |

## 6 Model quality i

### 6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts i

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 836   | 833      | 832      | 3±2     |
| All | All   | 16720 | 16660    | 16640    | 64      |

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 2.

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

| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:69:ASN:HD21 | 1:A:77:ILE:HD12  | 0.56     | 1.60        | 2      | 1     |
| 1:A:93:GLY:O    | 1:A:97:VAL:HG23  | 0.55     | 2.02        | 18     | 7     |
| 1:A:56:TYR:HB2  | 1:A:58:LYS:HE3   | 0.53     | 1.80        | 7      | 1     |
| 1:A:83:MET:N    | 1:A:83:MET:SD    | 0.52     | 2.82        | 8      | 4     |
| 1:A:62:LYS:HD3  | 1:A:62:LYS:O     | 0.51     | 2.05        | 9      | 2     |
| 1:A:69:ASN:HD21 | 1:A:77:ILE:HG23  | 0.51     | 1.65        | 12     | 1     |
| 1:A:83:MET:SD   | 1:A:83:MET:N     | 0.50     | 2.82        | 12     | 4     |
| 1:A:36:LYS:NZ   | 1:A:40:MET:SD    | 0.50     | 2.84        | 14     | 1     |
| 1:A:61:ALA:HB3  | 1:A:65:LYS:HB2   | 0.50     | 1.84        | 17     | 1     |
| 1:A:83:MET:O    | 1:A:83:MET:SD    | 0.49     | 2.70        | 15     | 1     |
| 1:A:71:LYS:HA   | 1:A:76:GLN:O     | 0.48     | 2.08        | 4      | 1     |
| 1:A:100:ASN:O   | 1:A:103:THR:HG22 | 0.47     | 2.08        | 18     | 2     |
| 1:A:92:ASN:O    | 1:A:95:LYS:HG2   | 0.47     | 2.09        | 12     | 1     |
| 1:A:27:ILE:HD12 | 1:A:97:VAL:HG22  | 0.47     | 1.85        | 14     | 3     |

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| Atom-1         | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|----------------|------------------|----------|-------------|--------|-------|
|                |                  |          |             | Worst  | Total |
| 1:A:69:ASN:ND2 | 1:A:77:ILE:HD12  | 0.45     | 2.26        | 2      | 1     |
| 1:A:97:VAL:O   | 1:A:101:GLY:N    | 0.45     | 2.49        | 14     | 1     |
| 1:A:65:LYS:CE  | 1:A:83:MET:SD    | 0.44     | 3.04        | 1      | 1     |
| 1:A:42:GLY:O   | 1:A:46:VAL:HG23  | 0.44     | 2.12        | 8      | 10    |
| 1:A:98:MET:O   | 1:A:102:LYS:HE3  | 0.43     | 2.13        | 18     | 1     |
| 1:A:53:GLU:O   | 1:A:56:TYR:CD2   | 0.42     | 2.72        | 1      | 1     |
| 1:A:72:ALA:HB3 | 1:A:76:GLN:HG2   | 0.42     | 1.90        | 2      | 4     |
| 1:A:47:GLN:NE2 | 1:A:104:THR:HA   | 0.42     | 2.28        | 8      | 1     |
| 1:A:58:LYS:N   | 1:A:58:LYS:HD3   | 0.42     | 2.30        | 4      | 1     |
| 1:A:92:ASN:HA  | 1:A:95:LYS:HE2   | 0.42     | 1.90        | 1      | 1     |
| 1:A:98:MET:O   | 1:A:102:LYS:HE2  | 0.42     | 2.15        | 1      | 1     |
| 1:A:3:GLY:HA3  | 1:A:20:LYS:O     | 0.42     | 2.15        | 8      | 1     |
| 1:A:21:ALA:O   | 1:A:23:ASN:N     | 0.42     | 2.53        | 17     | 2     |
| 1:A:50:SER:HB3 | 1:A:51:PRO:HD3   | 0.41     | 1.91        | 7      | 1     |
| 1:A:58:LYS:NZ  | 1:A:58:LYS:HB2   | 0.41     | 2.30        | 10     | 1     |
| 1:A:6:GLU:HB3  | 1:A:109:LEU:HD11 | 0.41     | 1.92        | 10     | 1     |
| 1:A:40:MET:HE2 | 1:A:43:ILE:HD12  | 0.41     | 1.91        | 5      | 1     |
| 1:A:49:ASN:OD1 | 1:A:55:ARG:NH1   | 0.41     | 2.54        | 1      | 1     |
| 1:A:16:LYS:N   | 1:A:16:LYS:HD3   | 0.40     | 2.31        | 18     | 1     |
| 1:A:102:LYS:NZ | 1:A:102:LYS:HB3  | 0.40     | 2.32        | 9      | 1     |
| 1:A:69:ASN:OD1 | 1:A:69:ASN:N     | 0.40     | 2.55        | 7      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured      | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|------------|-------------|----|
| 1   | A     | 109/118 (92%)   | 104±2 (96±1%) | 5±2 (4±1%) | 0±0 (0±0%) | 50          | 82 |
| All | All   | 2180/2360 (92%) | 2082 (96%)    | 94 (4%)    | 4 (0%)     | 50          | 82 |

All 2 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     | 22  | GLY  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 3   | GLY  | 1              |

### 6.3.2 Protein sidechains [i](#)

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1   | A     | 91/100 (91%)    | 89±1 (98±1%) | 2±1 (2±1%) | 53          | 92 |
| All | All   | 1820/2000 (91%) | 1778 (98%)   | 42 (2%)    | 53          | 92 |

All 17 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     | 16  | LYS  | 7              |
| 1   | A     | 58  | LYS  | 6              |
| 1   | A     | 83  | MET  | 5              |
| 1   | A     | 102 | LYS  | 4              |
| 1   | A     | 62  | LYS  | 3              |
| 1   | A     | 56  | TYR  | 3              |
| 1   | A     | 98  | MET  | 2              |
| 1   | A     | 63  | ASN  | 2              |
| 1   | A     | 90  | ARG  | 2              |
| 1   | A     | 20  | LYS  | 1              |
| 1   | A     | 82  | GLN  | 1              |
| 1   | A     | 44  | GLU  | 1              |
| 1   | A     | 9   | LYS  | 1              |
| 1   | A     | 31  | GLU  | 1              |
| 1   | A     | 99  | GLU  | 1              |
| 1   | A     | 41  | ASN  | 1              |
| 1   | A     | 65  | LYS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 87% 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 [i](#)

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                  | 1353 |
| Number of shifts mapped to atoms        | 1353 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 8    |

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action        |
|------------------------|----------|---------------------------------|-------------------------|
| $^{13}\text{C}_\alpha$ | 112      | $-0.58 \pm 0.22$                | Should be checked       |
| $^{13}\text{C}_\beta$  | 103      | $0.25 \pm 0.12$                 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$       | 107      | $-0.24 \pm 0.23$                | None needed (< 0.5 ppm) |
| $^{15}\text{N}$        | 109      | $0.46 \pm 0.56$                 | None needed (< 0.5 ppm) |

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1323 atoms were assigned a chemical shift out of a possible 1425. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 543/550 (99%) | 224/225 (100%) | 213/218 (98%)   | 106/107 (99%)   |
| Sidechain | 716/780 (92%) | 486/505 (96%)  | 216/245 (88%)   | 14/30 (47%)     |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 64/95 (67%)     | 32/45 (71%)    | 31/47 (66%)     | 1/3 (33%)       |
| Overall  | 1323/1425 (93%) | 742/775 (96%)  | 460/510 (90%)   | 121/140 (86%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1353 atoms were assigned a chemical shift out of a possible 1556. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 558/595 (94%)   | 230/243 (95%)  | 219/236 (93%)   | 109/116 (94%)   |
| Sidechain | 731/818 (89%)   | 496/530 (94%)  | 221/258 (86%)   | 14/30 (47%)     |
| Aromatic  | 64/143 (45%)    | 32/69 (46%)    | 31/59 (53%)     | 1/15 (7%)       |
| Overall   | 1353/1556 (87%) | 758/842 (90%)  | 471/553 (85%)   | 124/161 (77%)   |

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

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

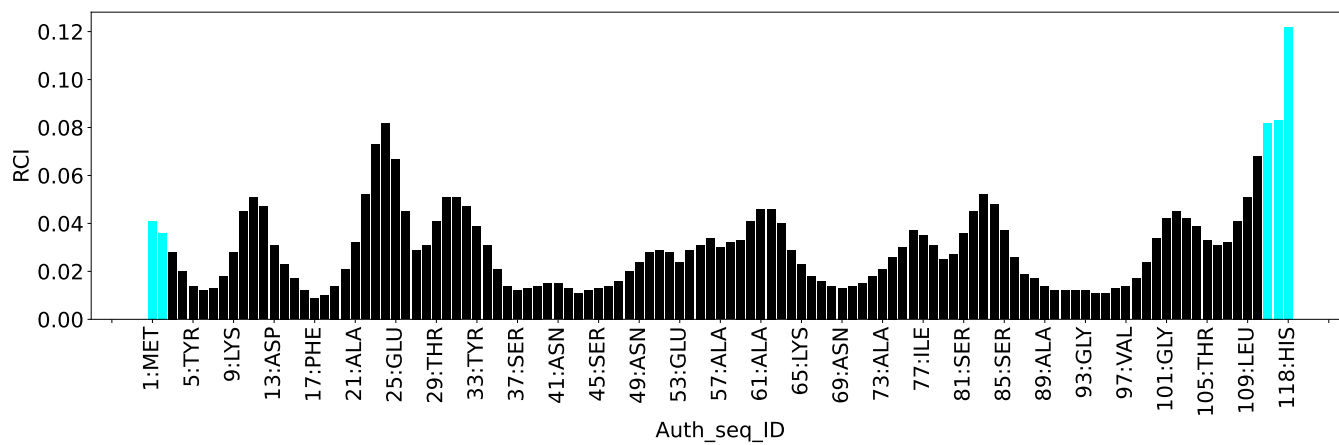
| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 59  | GLU  | HB3  | -0.39      | 0.95 – 3.05         | -11.4   |
| 1       | A     | 81  | SER  | HB2  | 1.43       | 2.61 – 5.13         | -9.7    |
| 1       | A     | 81  | SER  | HB3  | 1.43       | 2.49 – 5.20         | -8.9    |
| 1       | A     | 30  | SER  | HB3  | 1.50       | 2.49 – 5.20         | -8.7    |
| 1       | A     | 20  | LYS  | HB3  | -0.12      | 0.46 – 3.04         | -7.2    |
| 1       | A     | 43  | ILE  | HG13 | -0.99      | -0.82 – 3.23        | -5.4    |
| 1       | A     | 107 | LYS  | HE3  | 1.88       | 1.92 – 3.89         | -5.2    |
| 1       | A     | 20  | LYS  | HB2  | 0.58       | 0.58 – 2.97         | -5.0    |

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

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

Random coil index (RCI) for chain A:





## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description  | Value |
|--|-------|
| Total distance restraints                                | 2466  |
| Intra-residue ( $ i-j =0$ )                              | 564   |
| Sequential ( $ i-j =1$ )                                 | 567   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 414   |
| Long range ( $ i-j \geq 5$ )                             | 829   |
| Inter-chain  | 0     |
| Hydrogen bond restraints                                 | 92    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 146   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 22.1  |
| Number of long range restraints per residue <sup>1</sup> | 7.3   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|--|---------|
| 0.1-0.2 (Small)  | 8.0                                    | 0.2     |
| 0.2-0.5 (Medium) | 8.8                                    | 0.5     |
| >0.5 (Large)     | 80.7                                   | 5.63    |

### 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)   | 3.9                                    | 4.5     |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis [i](#)

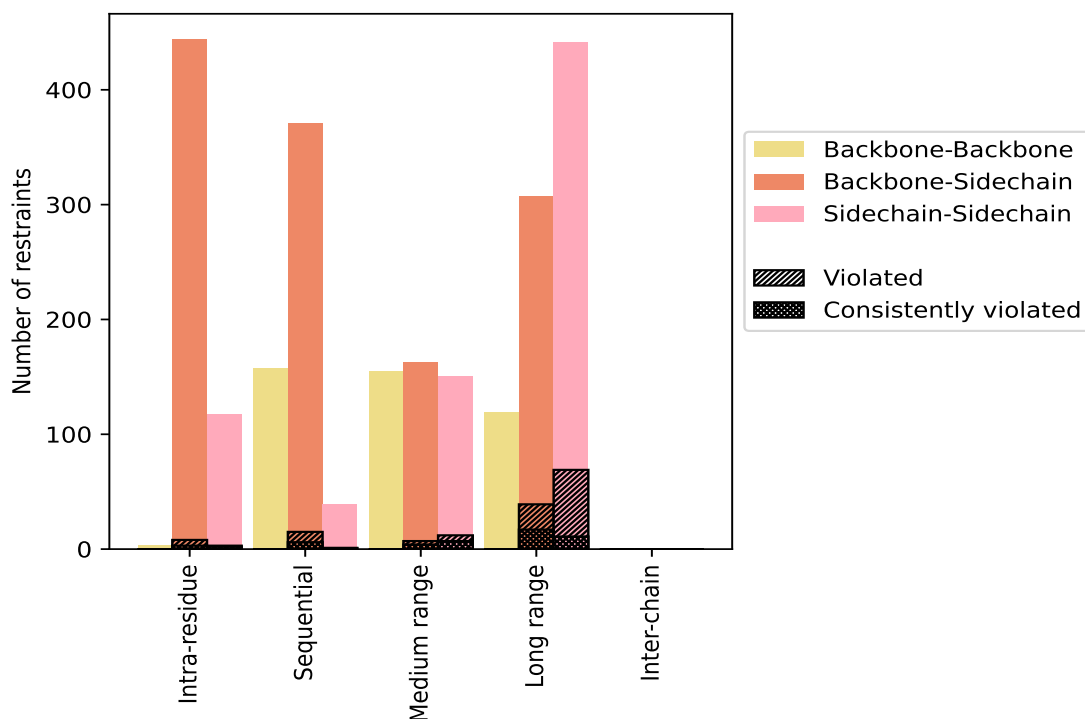
### 9.1 Summary of distance violations [i](#)

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

| 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>564</b>  | <b>22.9</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   | 3           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 444         | 18.0           | 8                     | 1.8            | 0.3            | 3                                  | 0.7            | 0.1            |
| Sidechain-Sidechain   | 117         | 4.7            | 3                     | 2.6            | 0.1            | 2                                  | 1.7            | 0.1            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>567</b>  | <b>23.0</b>    | <b>16</b>             | <b>2.8</b>     | <b>0.6</b>     | <b>7</b>                           | <b>1.2</b>     | <b>0.3</b>     |
| Backbone-Backbone   | 157         | 6.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 371         | 15.0           | 15                    | 4.0            | 0.6            | 6                                  | 1.6            | 0.2            |
| Sidechain-Sidechain   | 39          | 1.6            | 1                     | 2.6            | 0.0            | 1                                  | 2.6            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>414</b>  | <b>16.8</b>    | <b>19</b>             | <b>4.6</b>     | <b>0.8</b>     | <b>11</b>                          | <b>2.7</b>     | <b>0.4</b>     |
| Backbone-Backbone   | 101         | 4.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 163         | 6.6            | 7                     | 4.3            | 0.3            | 4                                  | 2.5            | 0.2            |
| Sidechain-Sidechain   | 150         | 6.1            | 12                    | 8.0            | 0.5            | 7                                  | 4.7            | 0.3            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>829</b>  | <b>33.6</b>    | <b>108</b>            | <b>13.0</b>    | <b>4.4</b>     | <b>28</b>                          | <b>3.4</b>     | <b>1.1</b>     |
| Backbone-Backbone   | 81          | 3.3            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 307         | 12.4           | 39                    | 12.7           | 1.6            | 17                                 | 5.5            | 0.7            |
| Sidechain-Sidechain   | 441         | 17.9           | 69                    | 15.6           | 2.8            | 11                                 | 2.5            | 0.4            |
| <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>92</b>   | <b>3.7</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>2466</b> | <b>100.0</b>   | <b>154</b>            | <b>6.2</b>     | <b>6.2</b>     | <b>51</b>                          | <b>2.1</b>     | <b>2.1</b>     |
| Backbone-Backbone   | 434         | 17.6           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 1285        | 52.1           | 69                    | 5.4            | 2.8            | 30                                 | 2.3            | 1.2            |
| Sidechain-Sidechain   | 747         | 30.3           | 85                    | 11.4           | 3.4            | 21                                 | 2.8            | 0.9            |

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid 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        | 7                    | 11              | 16              | 54              | 0               | 88    | 1.52     | 3.38    | 0.92                | 1.44       |
| 2        | 8                    | 11              | 11              | 58              | 0               | 88    | 1.48     | 3.19    | 0.92                | 1.37       |
| 3        | 10                   | 11              | 16              | 72              | 0               | 109   | 1.5      | 3.82    | 0.93                | 1.49       |
| 4        | 9                    | 11              | 15              | 72              | 0               | 107   | 1.53     | 3.62    | 0.9                 | 1.42       |
| 5        | 9                    | 10              | 11              | 56              | 0               | 86    | 1.56     | 3.45    | 0.9                 | 1.5        |
| 6        | 10                   | 12              | 15              | 72              | 0               | 109   | 1.47     | 3.43    | 0.88                | 1.44       |
| 7        | 10                   | 14              | 13              | 78              | 0               | 115   | 1.43     | 3.58    | 0.9                 | 1.21       |
| 8        | 8                    | 11              | 16              | 52              | 0               | 87    | 1.58     | 5.39    | 1.0                 | 1.57       |
| 9        | 8                    | 9               | 15              | 49              | 0               | 81    | 1.54     | 3.49    | 0.94                | 1.49       |
| 10       | 10                   | 11              | 13              | 73              | 0               | 107   | 1.6      | 4.0     | 0.98                | 1.47       |
| 11       | 11                   | 13              | 15              | 76              | 0               | 115   | 1.48     | 4.68    | 0.93                | 1.43       |

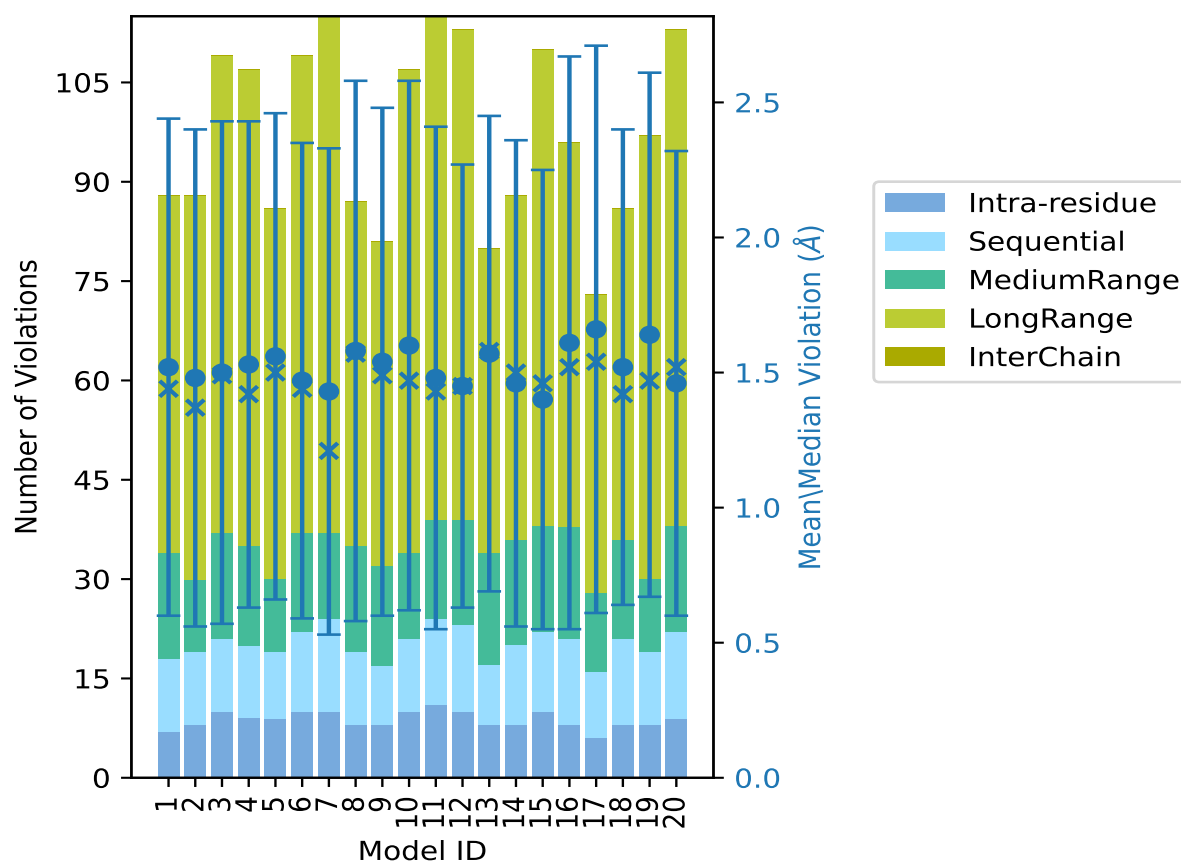
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| Model ID | Number of violations |                 |                 |                 |                 | Total | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> |       |          |         |                     |            |
| 12       | 10                   | 13              | 16              | 74              | 0               | 113   | 1.45     | 3.52    | 0.82                | 1.45       |
| 13       | 8                    | 9               | 17              | 46              | 0               | 80    | 1.57     | 3.44    | 0.88                | 1.58       |
| 14       | 8                    | 12              | 16              | 52              | 0               | 88    | 1.46     | 3.84    | 0.9                 | 1.5        |
| 15       | 10                   | 12              | 16              | 72              | 0               | 110   | 1.4      | 3.86    | 0.85                | 1.46       |
| 16       | 8                    | 13              | 17              | 58              | 0               | 96    | 1.61     | 5.63    | 1.06                | 1.52       |
| 17       | 6                    | 10              | 12              | 45              | 0               | 73    | 1.66     | 3.77    | 1.05                | 1.54       |
| 18       | 8                    | 13              | 15              | 50              | 0               | 86    | 1.52     | 3.35    | 0.88                | 1.42       |
| 19       | 8                    | 11              | 11              | 67              | 0               | 97    | 1.64     | 4.82    | 0.97                | 1.47       |
| 20       | 9                    | 13              | 16              | 75              | 0               | 113   | 1.46     | 3.58    | 0.86                | 1.52       |

<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 [i](#)



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

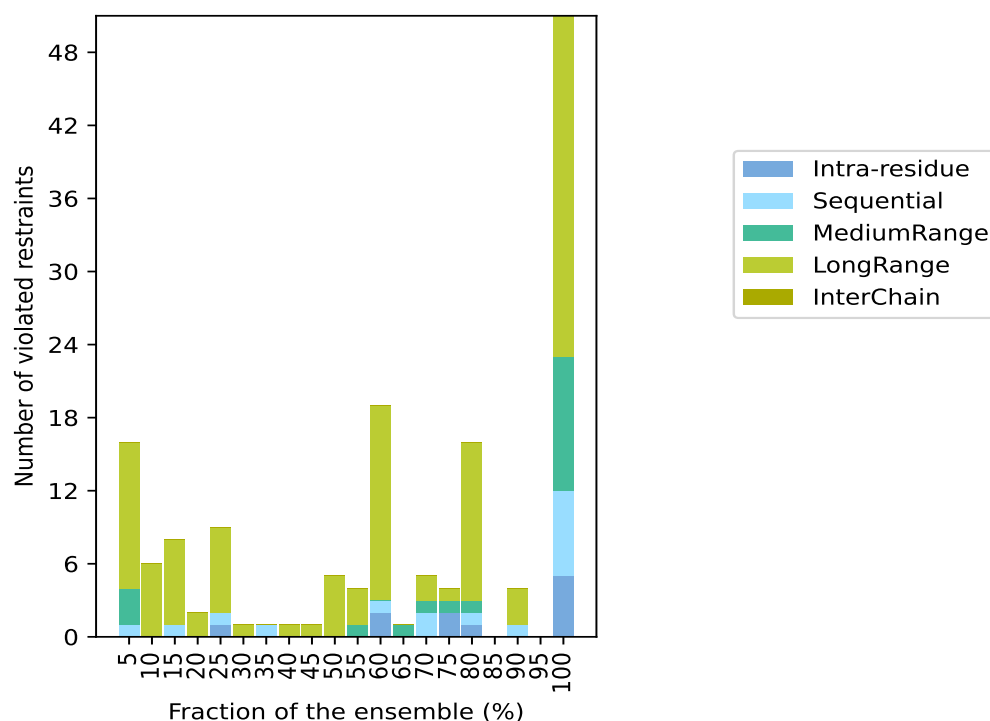
### 9.3 Distance violation statistics for the ensemble

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, 2220(IR:553, SQ:551, MR:395, LR:721, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 0                             | 1               | 3               | 12              | 0               | 16    | 1                        | 5.0   |
| 0                             | 0               | 0               | 6               | 0               | 6     | 2                        | 10.0  |
| 0                             | 1               | 0               | 7               | 0               | 8     | 3                        | 15.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 4                        | 20.0  |
| 1                             | 1               | 0               | 7               | 0               | 9     | 5                        | 25.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 6                        | 30.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 7                        | 35.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 8                        | 40.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 9                        | 45.0  |
| 0                             | 0               | 0               | 5               | 0               | 5     | 10                       | 50.0  |
| 0                             | 0               | 1               | 3               | 0               | 4     | 11                       | 55.0  |
| 2                             | 1               | 0               | 16              | 0               | 19    | 12                       | 60.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 13                       | 65.0  |
| 0                             | 2               | 1               | 2               | 0               | 5     | 14                       | 70.0  |
| 2                             | 0               | 1               | 1               | 0               | 4     | 15                       | 75.0  |
| 1                             | 1               | 1               | 13              | 0               | 16    | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 1               | 0               | 3               | 0               | 4     | 18                       | 90.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 19                       | 95.0  |
| 5                             | 7               | 11              | 28              | 0               | 51    | 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](#)

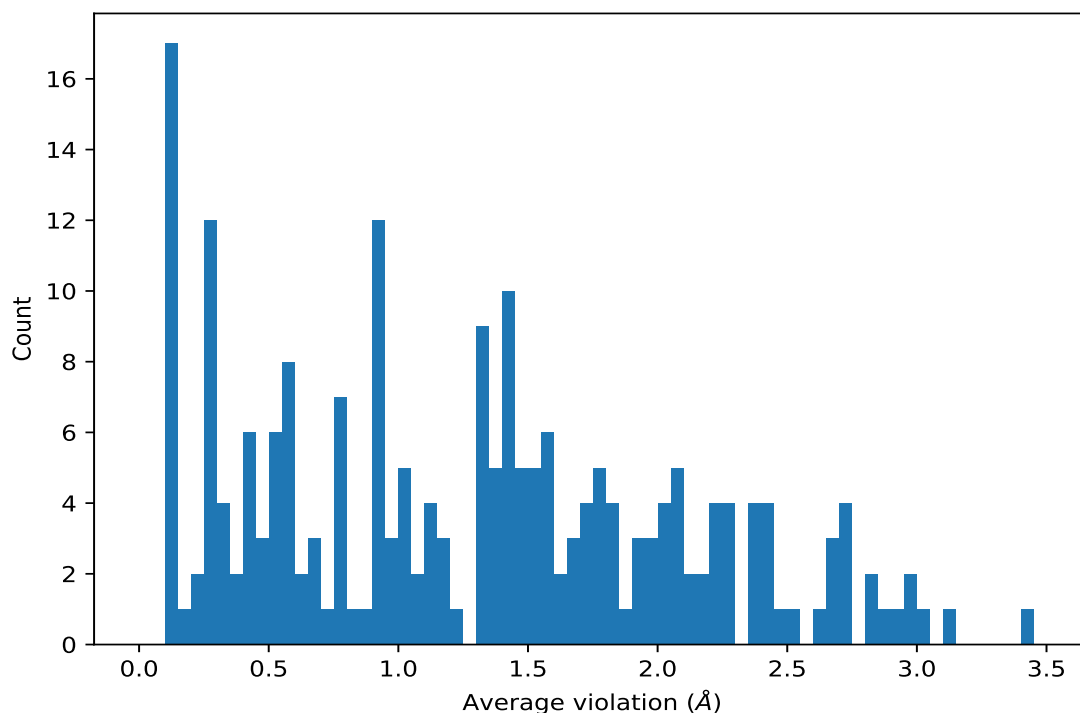


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1842) | 1:A:68:PHE:HE2  | 1:A:84:TYR:HE1 | 20                  | 3.41     | 1.06                | 3.46       |
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2 | 20                  | 3.1      | 0.38                | 3.1        |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2 | 20                  | 3.02     | 0.28                | 3.02       |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2 | 20                  | 2.96     | 0.31                | 3.0        |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2 | 20                  | 2.96     | 0.24                | 2.92       |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA  | 20                  | 2.92     | 0.2                 | 2.94       |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2 | 20                  | 2.9      | 0.41                | 2.72       |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H   | 20                  | 2.83     | 0.32                | 2.86       |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2 | 20                  | 2.73     | 0.19                | 2.72       |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2 | 20                  | 2.73     | 0.19                | 2.72       |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2 | 20                  | 2.73     | 0.19                | 2.72       |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2 | 20                  | 2.7      | 0.18                | 2.69       |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2 | 20                  | 2.67     | 0.09                | 2.67       |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2 | 20                  | 2.67     | 0.09                | 2.67       |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2 | 20                  | 2.67     | 0.09                | 2.67       |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2 | 20                  | 2.64     | 0.26                | 2.62       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 20                  | 2.47     | 0.27                | 2.48       |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 20                  | 2.44     | 0.25                | 2.47       |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 20                  | 2.44     | 0.25                | 2.49       |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 20                  | 2.42     | 0.3                 | 2.41       |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 20                  | 2.39     | 0.47                | 2.28       |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 20                  | 2.39     | 0.47                | 2.28       |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 20                  | 2.39     | 0.47                | 2.28       |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 20                  | 2.38     | 0.2                 | 2.32       |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2  | 20                  | 2.27     | 0.42                | 2.22       |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 20                  | 2.25     | 0.35                | 2.34       |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 20                  | 2.25     | 0.35                | 2.34       |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 20                  | 2.25     | 0.35                | 2.34       |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 20                  | 2.23     | 0.33                | 2.24       |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 20                  | 2.21     | 0.25                | 2.2        |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 20                  | 2.21     | 0.25                | 2.2        |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 20                  | 2.21     | 0.25                | 2.2        |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 20                  | 2.16     | 0.29                | 2.15       |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 20                  | 2.1      | 0.57                | 2.16       |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 20                  | 2.07     | 0.25                | 2.11       |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 20                  | 2.07     | 0.25                | 2.11       |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 20                  | 2.07     | 0.25                | 2.11       |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 20                  | 2.06     | 0.32                | 2.14       |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 20                  | 2.06     | 0.42                | 2.01       |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 20                  | 2.01     | 0.34                | 1.98       |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 20                  | 2.01     | 0.34                | 1.98       |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2  | 20                  | 1.98     | 0.23                | 1.95       |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2  | 20                  | 1.98     | 0.23                | 1.95       |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2  | 20                  | 1.98     | 0.23                | 1.95       |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 20                  | 1.92     | 0.56                | 1.92       |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 20                  | 1.92     | 0.56                | 1.92       |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 20                  | 1.92     | 0.56                | 1.92       |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 20                  | 1.81     | 0.55                | 1.96       |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 20                  | 1.81     | 0.55                | 1.96       |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 20                  | 1.81     | 0.55                | 1.96       |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2  | 20                  | 1.78     | 0.43                | 1.72       |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2  | 20                  | 1.71     | 0.46                | 1.82       |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2  | 20                  | 1.7      | 0.14                | 1.73       |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2  | 20                  | 1.61     | 0.32                | 1.61       |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2  | 20                  | 1.61     | 0.32                | 1.61       |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2  | 20                  | 1.57     | 0.28                | 1.6        |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2  | 20                  | 1.57     | 0.28                | 1.6        |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2  | 20                  | 1.57     | 0.28                | 1.6        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H    | 20                  | 1.35     | 0.35                | 1.3        |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H    | 20                  | 1.32     | 0.39                | 1.19       |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB2  | 20                  | 1.14     | 0.26                | 1.23       |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB3  | 20                  | 1.14     | 0.26                | 1.23       |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2  | 20                  | 1.13     | 0.14                | 1.08       |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H    | 20                  | 1.0      | 0.25                | 0.99       |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H    | 20                  | 0.96     | 0.09                | 0.96       |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 20                  | 0.95     | 0.31                | 0.95       |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2  | 20                  | 0.95     | 0.31                | 0.95       |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2  | 20                  | 0.95     | 0.31                | 0.95       |
| (1,1790) | 1:A:33:TYR:HD1  | 1:A:34:THR:H    | 20                  | 0.78     | 0.07                | 0.77       |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H    | 20                  | 0.77     | 0.11                | 0.81       |
| (1,1409) | 1:A:67:TYR:HD1  | 1:A:68:PHE:HA   | 20                  | 0.69     | 0.2                 | 0.78       |
| (1,468)  | 1:A:68:PHE:H    | 1:A:68:PHE:HD2  | 20                  | 0.6      | 0.1                 | 0.6        |
| (1,1807) | 1:A:67:TYR:H    | 1:A:67:TYR:HD2  | 20                  | 0.51     | 0.18                | 0.48       |
| (1,1413) | 1:A:68:PHE:HD1  | 1:A:69:ASN:HA   | 20                  | 0.36     | 0.12                | 0.38       |
| (1,1787) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HD1  | 20                  | 0.17     | 0.02                | 0.17       |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 20                  | 0.14     | 0.01                | 0.14       |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2  | 18                  | 0.98     | 0.41                | 1.13       |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3  | 18                  | 0.98     | 0.41                | 1.13       |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2  | 18                  | 0.9      | 0.79                | 0.77       |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3  | 18                  | 0.9      | 0.79                | 0.77       |
| (1,258)  | 1:A:15:PHE:H    | 1:A:33:TYR:HD2  | 18                  | 0.31     | 0.08                | 0.32       |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 18                  | 0.14     | 0.02                | 0.14       |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 18                  | 0.14     | 0.02                | 0.14       |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 16                  | 2.52     | 0.4                 | 2.5        |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1  | 16                  | 2.11     | 1.32                | 1.54       |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2  | 16                  | 2.04     | 0.43                | 2.09       |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3  | 16                  | 2.04     | 0.43                | 2.09       |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1  | 16                  | 1.77     | 0.47                | 1.76       |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1  | 16                  | 1.74     | 0.49                | 1.6        |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1  | 16                  | 1.73     | 0.57                | 1.62       |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2  | 16                  | 1.54     | 0.45                | 1.46       |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3  | 16                  | 1.54     | 0.45                | 1.46       |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1  | 16                  | 1.44     | 0.33                | 1.44       |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2  | 16                  | 1.44     | 0.33                | 1.44       |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3  | 16                  | 1.44     | 0.33                | 1.44       |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB1  | 16                  | 1.42     | 0.41                | 1.32       |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB2  | 16                  | 1.42     | 0.41                | 1.32       |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB3  | 16                  | 1.42     | 0.41                | 1.32       |
| (1,1407) | 1:A:67:TYR:HB3  | 1:A:84:TYR:HD1  | 16                  | 1.4      | 0.36                | 1.44       |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2  | 16                  | 1.36     | 0.54                | 1.41       |

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| Key      | Atom-1         | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2261) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HD3   | 16                  | 1.36     | 0.54                | 1.41       |
| (1,1385) | 1:A:66:PRO:HB2 | 1:A:84:TYR:HD1   | 16                  | 1.36     | 0.42                | 1.38       |
| (1,596)  | 1:A:84:TYR:HD2 | 1:A:85:SER:H     | 16                  | 1.03     | 0.16                | 1.01       |
| (1,1398) | 1:A:66:PRO:HG2 | 1:A:84:TYR:HD1   | 16                  | 0.75     | 0.35                | 0.8        |
| (1,1801) | 1:A:33:TYR:HE1 | 1:A:42:GLY:HA2   | 16                  | 0.64     | 0.3                 | 0.64       |
| (1,595)  | 1:A:84:TYR:H   | 1:A:84:TYR:HD1   | 16                  | 0.54     | 0.14                | 0.56       |
| (1,1844) | 1:A:81:SER:HB3 | 1:A:84:TYR:HE1   | 15                  | 1.73     | 0.6                 | 1.56       |
| (1,1550) | 1:A:84:TYR:HE2 | 1:A:89:ALA:HA    | 15                  | 0.78     | 0.34                | 0.72       |
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2   | 15                  | 0.24     | 0.09                | 0.22       |
| (1,1788) | 1:A:33:TYR:HB2 | 1:A:33:TYR:HD2   | 15                  | 0.12     | 0.01                | 0.12       |
| (1,928)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:HA    | 14                  | 1.52     | 0.05                | 1.52       |
| (1,26)   | 1:A:6:GLU:H    | 1:A:17:PHE:HD1   | 14                  | 1.32     | 0.2                 | 1.3        |
| (1,2245) | 1:A:81:SER:HB2 | 1:A:84:TYR:HE1   | 14                  | 1.3      | 0.72                | 1.47       |
| (1,2245) | 1:A:81:SER:HB3 | 1:A:84:TYR:HE1   | 14                  | 1.3      | 0.72                | 1.47       |
| (1,131)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:H     | 14                  | 1.05     | 0.03                | 1.04       |
| (1,842)  | 1:A:7:LEU:HD11 | 1:A:17:PHE:HD2   | 14                  | 0.33     | 0.09                | 0.34       |
| (1,842)  | 1:A:7:LEU:HD12 | 1:A:17:PHE:HD2   | 14                  | 0.33     | 0.09                | 0.34       |
| (1,842)  | 1:A:7:LEU:HD13 | 1:A:17:PHE:HD2   | 14                  | 0.33     | 0.09                | 0.34       |
| (1,1845) | 1:A:82:GLN:H   | 1:A:84:TYR:HE1   | 13                  | 0.46     | 0.37                | 0.29       |
| (1,115)  | 1:A:15:PHE:HD2 | 1:A:35:GLY:H     | 12                  | 2.82     | 0.38                | 2.8        |
| (1,1776) | 1:A:15:PHE:HD1 | 1:A:110:THR:HB   | 12                  | 2.42     | 0.29                | 2.45       |
| (1,1109) | 1:A:15:PHE:HD2 | 1:A:33:TYR:HB3   | 12                  | 2.17     | 0.21                | 2.19       |
| (1,859)  | 1:A:7:LEU:HG   | 1:A:15:PHE:HD1   | 12                  | 1.89     | 0.22                | 1.86       |
| (1,1780) | 1:A:15:PHE:HE1 | 1:A:110:THR:HB   | 12                  | 1.82     | 0.19                | 1.74       |
| (1,1721) | 1:A:15:PHE:HE1 | 1:A:110:THR:HG21 | 12                  | 1.78     | 0.13                | 1.76       |
| (1,1721) | 1:A:15:PHE:HE1 | 1:A:110:THR:HG22 | 12                  | 1.78     | 0.13                | 1.76       |
| (1,1721) | 1:A:15:PHE:HE1 | 1:A:110:THR:HG23 | 12                  | 1.78     | 0.13                | 1.76       |
| (1,1963) | 1:A:15:PHE:HE2 | 1:A:35:GLY:HA2   | 12                  | 1.67     | 0.32                | 1.63       |
| (1,1963) | 1:A:15:PHE:HE2 | 1:A:35:GLY:HA3   | 12                  | 1.67     | 0.32                | 1.63       |
| (1,1965) | 1:A:15:PHE:HD2 | 1:A:35:GLY:HA2   | 12                  | 1.57     | 0.32                | 1.5        |
| (1,1965) | 1:A:15:PHE:HD2 | 1:A:35:GLY:HA3   | 12                  | 1.57     | 0.32                | 1.5        |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG21 | 12                  | 1.49     | 0.06                | 1.47       |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG22 | 12                  | 1.49     | 0.06                | 1.47       |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG23 | 12                  | 1.49     | 0.06                | 1.47       |
| (1,879)  | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1   | 12                  | 1.42     | 0.53                | 1.31       |
| (1,2136) | 1:A:56:TYR:HB2 | 1:A:68:PHE:HD1   | 12                  | 1.32     | 0.61                | 1.38       |
| (1,2136) | 1:A:56:TYR:HB3 | 1:A:68:PHE:HD1   | 12                  | 1.32     | 0.61                | 1.38       |
| (1,852)  | 1:A:7:LEU:HD21 | 1:A:15:PHE:HD1   | 12                  | 1.3      | 0.37                | 1.2        |
| (1,852)  | 1:A:7:LEU:HD22 | 1:A:15:PHE:HD1   | 12                  | 1.3      | 0.37                | 1.2        |
| (1,852)  | 1:A:7:LEU:HD23 | 1:A:15:PHE:HD1   | 12                  | 1.3      | 0.37                | 1.2        |
| (1,114)  | 1:A:15:PHE:HD1 | 1:A:16:LYS:H     | 12                  | 1.06     | 0.06                | 1.08       |
| (1,838)  | 1:A:7:LEU:HD11 | 1:A:15:PHE:HD1   | 12                  | 1.0      | 0.17                | 0.96       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,838)  | 1:A:7:LEU:HD12  | 1:A:15:PHE:HD1   | 12                  | 1.0      | 0.17                | 0.96       |
| (1,838)  | 1:A:7:LEU:HD13  | 1:A:15:PHE:HD1   | 12                  | 1.0      | 0.17                | 0.96       |
| (1,113)  | 1:A:15:PHE:H    | 1:A:15:PHE:HD2   | 12                  | 0.95     | 0.06                | 0.94       |
| (1,1739) | 1:A:7:LEU:HD21  | 1:A:15:PHE:HE1   | 12                  | 0.94     | 0.36                | 0.8        |
| (1,1739) | 1:A:7:LEU:HD22  | 1:A:15:PHE:HE1   | 12                  | 0.94     | 0.36                | 0.8        |
| (1,1739) | 1:A:7:LEU:HD23  | 1:A:15:PHE:HE1   | 12                  | 0.94     | 0.36                | 0.8        |
| (1,117)  | 1:A:15:PHE:HE2  | 1:A:36:LYS:H     | 12                  | 0.86     | 0.3                 | 0.81       |
| (1,282)  | 1:A:15:PHE:HD2  | 1:A:36:LYS:H     | 12                  | 0.67     | 0.31                | 0.57       |
| (1,116)  | 1:A:15:PHE:H    | 1:A:15:PHE:HE2   | 12                  | 0.57     | 0.08                | 0.57       |
| (1,1843) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1   | 11                  | 1.59     | 0.66                | 1.46       |
| (1,877)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1   | 11                  | 1.15     | 0.41                | 0.99       |
| (1,1909) | 1:A:9:LYS:HB2   | 1:A:15:PHE:HE1   | 11                  | 0.75     | 0.39                | 0.58       |
| (1,1909) | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1   | 11                  | 0.75     | 0.39                | 0.58       |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG21  | 11                  | 0.28     | 0.19                | 0.17       |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG22  | 11                  | 0.28     | 0.19                | 0.17       |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG23  | 11                  | 0.28     | 0.19                | 0.17       |
| (1,470)  | 1:A:68:PHE:HE2  | 1:A:94:ILE:H     | 10                  | 0.85     | 0.86                | 0.36       |
| (1,887)  | 1:A:9:LYS:HG2   | 1:A:15:PHE:HE1   | 10                  | 0.65     | 0.52                | 0.51       |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG21  | 10                  | 0.55     | 0.23                | 0.48       |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG22  | 10                  | 0.55     | 0.23                | 0.48       |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG23  | 10                  | 0.55     | 0.23                | 0.48       |
| (1,1828) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB2   | 10                  | 0.54     | 0.27                | 0.6        |
| (1,1773) | 1:A:9:LYS:HA    | 1:A:15:PHE:HD1   | 10                  | 0.41     | 0.17                | 0.4        |
| (1,1497) | 1:A:27:ILE:HD11 | 1:A:97:VAL:HB    | 9                   | 0.13     | 0.02                | 0.14       |
| (1,1497) | 1:A:27:ILE:HD12 | 1:A:97:VAL:HB    | 9                   | 0.13     | 0.02                | 0.14       |
| (1,1497) | 1:A:27:ILE:HD13 | 1:A:97:VAL:HB    | 9                   | 0.13     | 0.02                | 0.14       |
| (1,1908) | 1:A:9:LYS:HB2   | 1:A:15:PHE:HD1   | 8                   | 0.56     | 0.35                | 0.41       |
| (1,1908) | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1   | 8                   | 0.56     | 0.35                | 0.41       |
| (1,850)  | 1:A:7:LEU:HD21  | 1:A:8:SER:HA     | 7                   | 0.12     | 0.01                | 0.12       |
| (1,850)  | 1:A:7:LEU:HD22  | 1:A:8:SER:HA     | 7                   | 0.12     | 0.01                | 0.12       |
| (1,850)  | 1:A:7:LEU:HD23  | 1:A:8:SER:HA     | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1799) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA3   | 6                   | 0.28     | 0.13                | 0.25       |
| (1,1884) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HB2   | 5                   | 1.46     | 0.07                | 1.48       |
| (1,1884) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HB3   | 5                   | 1.46     | 0.07                | 1.48       |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG21 | 5                   | 1.45     | 0.55                | 1.25       |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG22 | 5                   | 1.45     | 0.55                | 1.25       |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG23 | 5                   | 1.45     | 0.55                | 1.25       |
| (1,1180) | 1:A:5:TYR:HD2   | 1:A:43:ILE:HG13  | 5                   | 1.16     | 0.27                | 1.11       |
| (1,37)   | 1:A:5:TYR:HD2   | 1:A:6:GLU:H      | 5                   | 0.91     | 0.05                | 0.92       |
| (1,36)   | 1:A:5:TYR:H     | 1:A:5:TYR:HD1    | 5                   | 0.73     | 0.05                | 0.75       |
| (1,878)  | 1:A:9:LYS:HB2   | 1:A:15:PHE:HE1   | 5                   | 0.63     | 0.3                 | 0.77       |
| (1,1823) | 1:A:68:PHE:HE2  | 1:A:81:SER:HB3   | 5                   | 0.54     | 0.55                | 0.2        |

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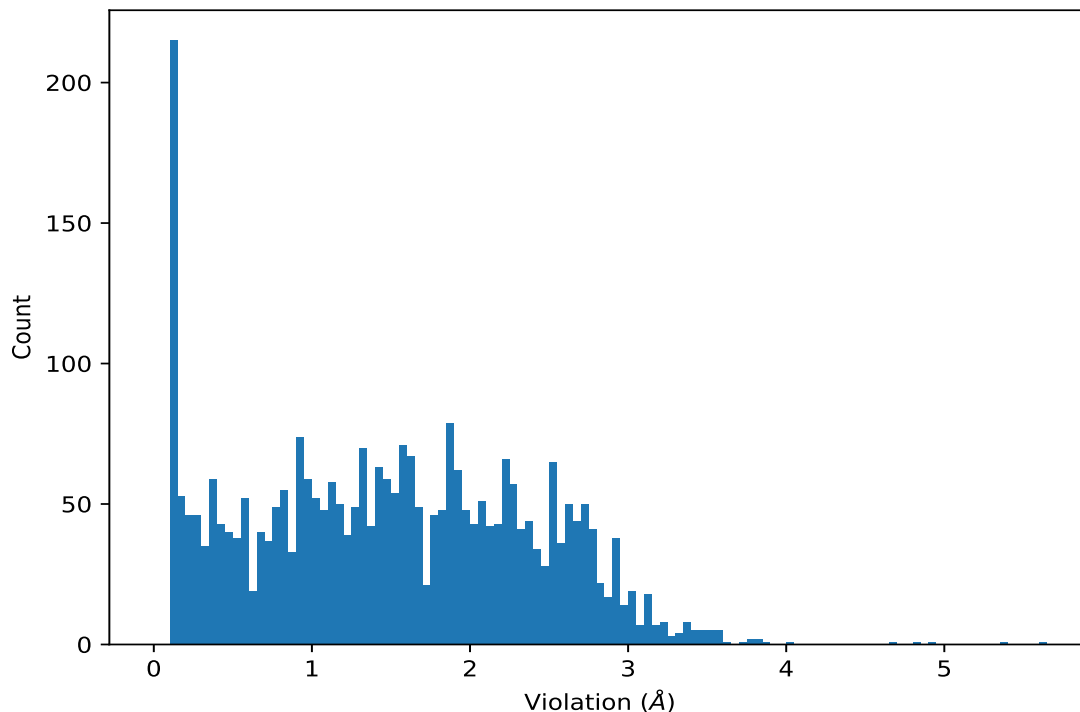
| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1885) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HG12 | 5                   | 0.44     | 0.24                | 0.37       |
| (1,1885) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HG13 | 5                   | 0.44     | 0.24                | 0.37       |
| (1,1927) | 1:A:9:LYS:HE2  | 1:A:15:PHE:HE1  | 5                   | 0.29     | 0.12                | 0.37       |
| (1,1927) | 1:A:9:LYS:HE3  | 1:A:15:PHE:HE1  | 5                   | 0.29     | 0.12                | 0.37       |
| (1,2200) | 1:A:68:PHE:HE2 | 1:A:93:GLY:HA2  | 4                   | 1.54     | 0.77                | 1.62       |
| (1,2200) | 1:A:68:PHE:HE2 | 1:A:93:GLY:HA3  | 4                   | 1.54     | 0.77                | 1.62       |
| (1,1822) | 1:A:68:PHE:HE2 | 1:A:81:SER:HB2  | 4                   | 0.6      | 0.42                | 0.43       |
| (1,1554) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HA   | 3                   | 0.76     | 0.13                | 0.8        |
| (1,2202) | 1:A:68:PHE:HD2 | 1:A:81:SER:HB2  | 3                   | 0.54     | 0.37                | 0.45       |
| (1,2202) | 1:A:68:PHE:HD2 | 1:A:81:SER:HB3  | 3                   | 0.54     | 0.37                | 0.45       |
| (1,1840) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HA   | 3                   | 0.42     | 0.24                | 0.38       |
| (1,1803) | 1:A:33:TYR:HE1 | 1:A:39:ALA:HA   | 3                   | 0.42     | 0.16                | 0.45       |
| (1,876)  | 1:A:9:LYS:HB2  | 1:A:15:PHE:HD1  | 3                   | 0.39     | 0.07                | 0.38       |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG11 | 3                   | 0.25     | 0.13                | 0.21       |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG12 | 3                   | 0.25     | 0.13                | 0.21       |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG13 | 3                   | 0.25     | 0.13                | 0.21       |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG21 | 3                   | 0.25     | 0.13                | 0.21       |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG22 | 3                   | 0.25     | 0.13                | 0.21       |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG23 | 3                   | 0.25     | 0.13                | 0.21       |
| (1,462)  | 1:A:67:TYR:HD2 | 1:A:84:TYR:H    | 3                   | 0.21     | 0.01                | 0.21       |
| (1,987)  | 1:A:21:ALA:HB1 | 1:A:22:GLY:H    | 3                   | 0.15     | 0.01                | 0.15       |
| (1,987)  | 1:A:21:ALA:HB2 | 1:A:22:GLY:H    | 3                   | 0.15     | 0.01                | 0.15       |
| (1,987)  | 1:A:21:ALA:HB3 | 1:A:22:GLY:H    | 3                   | 0.15     | 0.01                | 0.15       |
| (1,1829) | 1:A:68:PHE:HD2 | 1:A:81:SER:HB3  | 2                   | 1.21     | 0.24                | 1.21       |
| (1,2199) | 1:A:68:PHE:HE2 | 1:A:81:SER:HB2  | 2                   | 1.17     | 0.45                | 1.17       |
| (1,2199) | 1:A:68:PHE:HE2 | 1:A:81:SER:HB3  | 2                   | 1.17     | 0.45                | 1.17       |
| (1,1923) | 1:A:9:LYS:HD2  | 1:A:15:PHE:HE1  | 2                   | 0.94     | 0.11                | 0.94       |
| (1,1923) | 1:A:9:LYS:HD3  | 1:A:15:PHE:HE1  | 2                   | 0.94     | 0.11                | 0.94       |
| (1,1917) | 1:A:9:LYS:HG2  | 1:A:15:PHE:HE1  | 2                   | 0.48     | 0.21                | 0.48       |
| (1,1917) | 1:A:9:LYS:HG3  | 1:A:15:PHE:HE1  | 2                   | 0.48     | 0.21                | 0.48       |
| (1,1588) | 1:A:68:PHE:HD2 | 1:A:94:ILE:HG13 | 2                   | 0.44     | 0.09                | 0.44       |
| (1,2185) | 1:A:65:LYS:HD2 | 1:A:83:MET:HB2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,2185) | 1:A:65:LYS:HD2 | 1:A:83:MET:HB3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,2185) | 1:A:65:LYS:HD3 | 1:A:83:MET:HB2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,2185) | 1:A:65:LYS:HD3 | 1:A:83:MET:HB3  | 2                   | 0.14     | 0.01                | 0.14       |

<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) |
|----------|----------------|----------------|----------|---------------|
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1 | 16       | 5.63          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1 | 8        | 5.39          |
| (1,1770) | 1:A:5:TYR:HD2  | 1:A:17:PHE:HD1 | 16       | 4.9           |
| (1,1770) | 1:A:5:TYR:HD2  | 1:A:17:PHE:HD1 | 19       | 4.82          |
| (1,1770) | 1:A:5:TYR:HD2  | 1:A:17:PHE:HD1 | 11       | 4.68          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1 | 10       | 4.0           |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1 | 15       | 3.86          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1 | 14       | 3.84          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1 | 3        | 3.82          |
| (1,1815) | 1:A:61:ALA:HA  | 1:A:67:TYR:HE2 | 17       | 3.77          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1781) | 1:A:16:LYS:HB2 | 1:A:33:TYR:HD2  | 10       | 3.77          |
| (1,1815) | 1:A:61:ALA:HA  | 1:A:67:TYR:HE2  | 19       | 3.73          |
| (1,1781) | 1:A:16:LYS:HB2 | 1:A:33:TYR:HD2  | 4        | 3.62          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1  | 20       | 3.58          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG21 | 7        | 3.58          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG22 | 7        | 3.58          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG23 | 7        | 3.58          |
| (1,1400) | 1:A:67:TYR:HA  | 1:A:84:TYR:HD1  | 16       | 3.56          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1  | 12       | 3.52          |
| (1,1794) | 1:A:16:LYS:HA  | 1:A:33:TYR:HE2  | 4        | 3.52          |
| (1,1781) | 1:A:16:LYS:HB2 | 1:A:33:TYR:HD2  | 7        | 3.52          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1  | 17       | 3.5           |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1  | 19       | 3.5           |
| (1,1815) | 1:A:61:ALA:HA  | 1:A:67:TYR:HE2  | 9        | 3.49          |
| (1,115)  | 1:A:15:PHE:HD2 | 1:A:35:GLY:H    | 12       | 3.49          |
| (1,1794) | 1:A:16:LYS:HA  | 1:A:33:TYR:HE2  | 5        | 3.45          |
| (1,1794) | 1:A:16:LYS:HA  | 1:A:33:TYR:HE2  | 10       | 3.45          |
| (1,1781) | 1:A:16:LYS:HB2 | 1:A:33:TYR:HD2  | 9        | 3.45          |
| (1,1781) | 1:A:16:LYS:HB2 | 1:A:33:TYR:HD2  | 13       | 3.44          |
| (1,1783) | 1:A:17:PHE:H   | 1:A:33:TYR:HD2  | 6        | 3.43          |
| (1,1815) | 1:A:61:ALA:HA  | 1:A:67:TYR:HE2  | 10       | 3.42          |
| (1,1795) | 1:A:17:PHE:H   | 1:A:33:TYR:HE2  | 4        | 3.42          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1  | 11       | 3.41          |
| (1,1795) | 1:A:17:PHE:H   | 1:A:33:TYR:HE2  | 5        | 3.39          |
| (1,1795) | 1:A:17:PHE:H   | 1:A:33:TYR:HE2  | 6        | 3.39          |
| (1,1781) | 1:A:16:LYS:HB2 | 1:A:33:TYR:HD2  | 11       | 3.39          |
| (1,1412) | 1:A:67:TYR:HD1 | 1:A:69:ASN:HA   | 1        | 3.38          |
| (1,115)  | 1:A:15:PHE:HD2 | 1:A:35:GLY:H    | 10       | 3.38          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1  | 6        | 3.36          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1  | 18       | 3.35          |
| (1,1794) | 1:A:16:LYS:HA  | 1:A:33:TYR:HE2  | 7        | 3.35          |
| (1,1400) | 1:A:67:TYR:HA  | 1:A:84:TYR:HD1  | 8        | 3.34          |
| (1,1783) | 1:A:17:PHE:H   | 1:A:33:TYR:HD2  | 11       | 3.33          |
| (1,1781) | 1:A:16:LYS:HB2 | 1:A:33:TYR:HD2  | 5        | 3.32          |
| (1,1781) | 1:A:16:LYS:HB2 | 1:A:33:TYR:HD2  | 17       | 3.32          |
| (1,1811) | 1:A:67:TYR:HD1 | 1:A:81:SER:H    | 17       | 3.3           |
| (1,1794) | 1:A:16:LYS:HA  | 1:A:33:TYR:HE2  | 1        | 3.3           |
| (1,1795) | 1:A:17:PHE:H   | 1:A:33:TYR:HE2  | 10       | 3.29          |
| (1,1795) | 1:A:17:PHE:H   | 1:A:33:TYR:HE2  | 1        | 3.24          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1  | 13       | 3.23          |
| (1,1783) | 1:A:17:PHE:H   | 1:A:33:TYR:HD2  | 10       | 3.23          |
| (1,1795) | 1:A:17:PHE:H   | 1:A:33:TYR:HE2  | 11       | 3.21          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2 | 8        | 3.21          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2 | 20       | 3.2           |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2 | 5        | 3.2           |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2 | 20       | 3.2           |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2 | 2        | 3.19          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2 | 4        | 3.19          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA  | 8        | 3.19          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H   | 7        | 3.17          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H   | 14       | 3.17          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2 | 17       | 3.16          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA  | 18       | 3.16          |
| (1,1842) | 1:A:68:PHE:HE2  | 1:A:84:TYR:HE1 | 7        | 3.15          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H   | 1        | 3.15          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2 | 19       | 3.15          |
| (1,1842) | 1:A:68:PHE:HE2  | 1:A:84:TYR:HE1 | 1        | 3.14          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2 | 4        | 3.14          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2 | 5        | 3.13          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H   | 18       | 3.12          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2 | 6        | 3.12          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2 | 15       | 3.12          |
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2 | 20       | 3.12          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2 | 7        | 3.11          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2 | 20       | 3.11          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2 | 9        | 3.11          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2 | 2        | 3.1           |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2 | 10       | 3.1           |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2 | 10       | 3.1           |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2 | 10       | 3.1           |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2 | 2        | 3.1           |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1 | 8        | 3.09          |
| (1,1843) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1 | 16       | 3.08          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2 | 11       | 3.08          |
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2 | 3        | 3.08          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2 | 15       | 3.06          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA  | 14       | 3.06          |
| (1,115)  | 1:A:15:PHE:HD2  | 1:A:35:GLY:H   | 6        | 3.06          |
| (1,1842) | 1:A:68:PHE:HE2  | 1:A:84:TYR:HE1 | 4        | 3.05          |
| (1,1842) | 1:A:68:PHE:HE2  | 1:A:84:TYR:HE1 | 9        | 3.04          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H   | 3        | 3.04          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H   | 16       | 3.04          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2 | 17       | 3.04          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2 | 13       | 3.04          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,115)  | 1:A:15:PHE:HD2  | 1:A:35:GLY:H   | 11       | 3.04          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2 | 2        | 3.03          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA  | 6        | 3.03          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA  | 11       | 3.03          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2 | 2        | 3.02          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2 | 19       | 3.02          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA  | 17       | 3.02          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2 | 3        | 3.01          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2 | 8        | 3.01          |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1 | 16       | 3.0           |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H   | 12       | 3.0           |
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2 | 19       | 3.0           |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA  | 9        | 3.0           |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2 | 8        | 2.99          |
| (1,115)  | 1:A:15:PHE:HD2  | 1:A:35:GLY:H   | 3        | 2.99          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA  | 10       | 2.98          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1 | 16       | 2.97          |
| (1,1776) | 1:A:15:PHE:HD1  | 1:A:110:THR:HB | 10       | 2.97          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H   | 11       | 2.96          |
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2 | 15       | 2.96          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA  | 3        | 2.96          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2 | 10       | 2.95          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3 | 10       | 2.95          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2 | 2        | 2.95          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2 | 2        | 2.95          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2 | 1        | 2.95          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2 | 3        | 2.95          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2 | 17       | 2.94          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3 | 17       | 2.94          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2 | 8        | 2.94          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2 | 14       | 2.94          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2 | 17       | 2.94          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2 | 4        | 2.93          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2 | 4        | 2.93          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2 | 4        | 2.93          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2 | 17       | 2.93          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2 | 7        | 2.93          |
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2 | 14       | 2.93          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2 | 9        | 2.93          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA  | 2        | 2.93          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2 | 4        | 2.93          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2 | 18       | 2.92          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 18       | 2.92          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 18       | 2.92          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 19       | 2.92          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 4        | 2.92          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2  | 1        | 2.92          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2  | 17       | 2.92          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 2        | 2.92          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 1        | 2.92          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 1        | 2.92          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 1        | 2.92          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 18       | 2.92          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 18       | 2.92          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 18       | 2.92          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 19       | 2.91          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 19       | 2.91          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 19       | 2.91          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 20       | 2.91          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 20       | 2.91          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 20       | 2.91          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2  | 20       | 2.91          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 14       | 2.91          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 14       | 2.91          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 14       | 2.91          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 17       | 2.9           |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 17       | 2.9           |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 17       | 2.9           |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2  | 19       | 2.89          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H    | 6        | 2.88          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 18       | 2.88          |
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2  | 6        | 2.88          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA   | 16       | 2.88          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 10       | 2.87          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2  | 16       | 2.86          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA   | 19       | 2.86          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 3        | 2.86          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H    | 8        | 2.85          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 10       | 2.85          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2  | 15       | 2.85          |
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2  | 1        | 2.85          |
| (1,115)  | 1:A:15:PHE:HD2  | 1:A:35:GLY:H    | 19       | 2.85          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2  | 9        | 2.84          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 10       | 2.84          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2  | 9        | 2.84          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 13       | 2.83          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 13       | 2.83          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 13       | 2.83          |
| (1,2245) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1  | 16       | 2.83          |
| (1,2245) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1  | 16       | 2.83          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 16       | 2.83          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2  | 13       | 2.83          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA   | 5        | 2.83          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 1        | 2.82          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 1        | 2.82          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 1        | 2.82          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 1        | 2.82          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 7        | 2.81          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 7        | 2.81          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 7        | 2.81          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1  | 8        | 2.81          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2  | 3        | 2.81          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA   | 7        | 2.81          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 17       | 2.81          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 7        | 2.8           |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 7        | 2.8           |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 7        | 2.8           |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 3        | 2.8           |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2  | 16       | 2.8           |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2  | 19       | 2.8           |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 6        | 2.79          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 6        | 2.79          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 6        | 2.79          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 15       | 2.79          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 4        | 2.79          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 15       | 2.79          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2  | 17       | 2.79          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 1        | 2.79          |
| (1,1776) | 1:A:15:PHE:HD1  | 1:A:110:THR:HB  | 6        | 2.78          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 4        | 2.78          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 4        | 2.78          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 4        | 2.78          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 5        | 2.78          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 5        | 2.78          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 5        | 2.78          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H    | 5        | 2.77          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 6        | 2.77          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2  | 16       | 2.77          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 7        | 2.77          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 7        | 2.77          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 7        | 2.77          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1  | 8        | 2.77          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 19       | 2.76          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 19       | 2.76          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 19       | 2.76          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 8        | 2.76          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 8        | 2.76          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 8        | 2.76          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 18       | 2.75          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 18       | 2.75          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 18       | 2.75          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 4        | 2.75          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 2        | 2.75          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 2        | 2.75          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 2        | 2.75          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 1        | 2.74          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 1        | 2.74          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 1        | 2.74          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2  | 13       | 2.74          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 17       | 2.74          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2  | 12       | 2.74          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 9        | 2.74          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 9        | 2.74          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 9        | 2.74          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA   | 15       | 2.74          |
| (1,115)  | 1:A:15:PHE:HD2  | 1:A:35:GLY:H    | 15       | 2.74          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 4        | 2.73          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 15       | 2.73          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 15       | 2.73          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 15       | 2.73          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 13       | 2.73          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2  | 19       | 2.73          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 16       | 2.73          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 10       | 2.73          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 7        | 2.72          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 5        | 2.72          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 5        | 2.72          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 5        | 2.72          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 12       | 2.72          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 12       | 2.72          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 12       | 2.72          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 3        | 2.72          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2  | 13       | 2.72          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 9        | 2.72          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 11       | 2.72          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA   | 13       | 2.72          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 14       | 2.72          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2  | 18       | 2.71          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 10       | 2.71          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1  | 16       | 2.71          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 3        | 2.71          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 3        | 2.71          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 3        | 2.71          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 6        | 2.7           |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 10       | 2.7           |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H    | 4        | 2.7           |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H    | 19       | 2.7           |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 9        | 2.7           |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2  | 16       | 2.7           |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 19       | 2.7           |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 19       | 2.7           |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 19       | 2.7           |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 6        | 2.7           |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 6        | 2.7           |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 6        | 2.7           |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 17       | 2.69          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2  | 4        | 2.69          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 17       | 2.69          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 7        | 2.69          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2  | 18       | 2.69          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 20       | 2.69          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 20       | 2.69          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 20       | 2.69          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2  | 19       | 2.68          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3  | 19       | 2.68          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H    | 13       | 2.68          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 5        | 2.68          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 3        | 2.68          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 18       | 2.68          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 13       | 2.68          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 13       | 2.68          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 13       | 2.68          |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 3        | 2.68          |
| (1,115)  | 1:A:15:PHE:HD2  | 1:A:35:GLY:H    | 4        | 2.68          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 9        | 2.67          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 9        | 2.67          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 9        | 2.67          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H    | 10       | 2.67          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 20       | 2.67          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 5        | 2.67          |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 15       | 2.67          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 3        | 2.66          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 3        | 2.66          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 3        | 2.66          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 4        | 2.66          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2  | 7        | 2.66          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2  | 8        | 2.66          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 14       | 2.66          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 14       | 2.66          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 14       | 2.66          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 14       | 2.66          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 19       | 2.66          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 19       | 2.66          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 19       | 2.66          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 9        | 2.66          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 9        | 2.66          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 9        | 2.66          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA   | 12       | 2.66          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 18       | 2.66          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 18       | 2.65          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 18       | 2.65          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 18       | 2.65          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2  | 10       | 2.65          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 3        | 2.65          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 3        | 2.65          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 3        | 2.65          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 6        | 2.65          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 6        | 2.65          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 6        | 2.65          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA   | 4        | 2.65          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 1        | 2.64          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2  | 14       | 2.64          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2  | 2        | 2.64          |
| (1,1776) | 1:A:15:PHE:HD1  | 1:A:110:THR:HB  | 2        | 2.64          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 10       | 2.64          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 16       | 2.63          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 14       | 2.63          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 14       | 2.63          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 14       | 2.63          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2  | 15       | 2.63          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 18       | 2.63          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 19       | 2.63          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2  | 1        | 2.63          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 17       | 2.63          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 17       | 2.63          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 17       | 2.63          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1  | 16       | 2.63          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H    | 2        | 2.62          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2  | 18       | 2.62          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2  | 12       | 2.62          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 17       | 2.62          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 16       | 2.62          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 16       | 2.62          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 16       | 2.62          |
| (1,1109) | 1:A:15:PHE:HD2  | 1:A:33:TYR:HB3  | 12       | 2.62          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 11       | 2.61          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 11       | 2.61          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 11       | 2.61          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 18       | 2.61          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 20       | 2.61          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 10       | 2.61          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 10       | 2.61          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 10       | 2.61          |
| (1,115)  | 1:A:15:PHE:HD2  | 1:A:35:GLY:H    | 5        | 2.61          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2  | 12       | 2.6           |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 6        | 2.6           |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 19       | 2.6           |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 4        | 2.6           |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 18       | 2.6           |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 11       | 2.59          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 7        | 2.59          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 13       | 2.59          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 3        | 2.59          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 3        | 2.59          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 3        | 2.59          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 12       | 2.59          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 12       | 2.59          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 12       | 2.59          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 7        | 2.58          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 17       | 2.58          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 17       | 2.58          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 17       | 2.58          |
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2  | 16       | 2.58          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 6        | 2.58          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 6        | 2.58          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 6        | 2.58          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 1        | 2.57          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 1        | 2.57          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 1        | 2.57          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 2        | 2.57          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 2        | 2.57          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 2        | 2.57          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 10       | 2.57          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H    | 9        | 2.57          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2  | 3        | 2.57          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 8        | 2.57          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 7        | 2.57          |
| (1,1794) | 1:A:16:LYS:HA   | 1:A:33:TYR:HE2  | 18       | 2.56          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2  | 14       | 2.56          |
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2  | 12       | 2.56          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 7        | 2.56          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2  | 1        | 2.56          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 11       | 2.56          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 11       | 2.56          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 11       | 2.56          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 5        | 2.55          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 4        | 2.55          |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 11       | 2.55          |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 14       | 2.55          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2  | 11       | 2.54          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3  | 11       | 2.54          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 4        | 2.54          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 17       | 2.54          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 2        | 2.54          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 20       | 2.54          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 15       | 2.54          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2   | 15       | 2.54          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2   | 15       | 2.54          |
| (1,1412) | 1:A:67:TYR:HD1  | 1:A:69:ASN:HA    | 20       | 2.54          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2   | 2        | 2.53          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3   | 5        | 2.53          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3   | 9        | 2.53          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3   | 16       | 2.53          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2   | 5        | 2.53          |
| (1,1776) | 1:A:15:PHE:HD1  | 1:A:110:THR:HB   | 19       | 2.53          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2   | 3        | 2.53          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2   | 9        | 2.53          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2   | 7        | 2.52          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2   | 10       | 2.52          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2   | 10       | 2.52          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2   | 10       | 2.52          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2   | 19       | 2.52          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2   | 19       | 2.52          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2   | 19       | 2.52          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2   | 2        | 2.52          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 10       | 2.52          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2   | 12       | 2.52          |
| (1,1776) | 1:A:15:PHE:HD1  | 1:A:110:THR:HB   | 5        | 2.52          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2   | 5        | 2.52          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2   | 20       | 2.52          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11  | 2        | 2.52          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12  | 2        | 2.52          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13  | 2        | 2.52          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11  | 11       | 2.52          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12  | 11       | 2.52          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13  | 11       | 2.52          |
| (1,115)  | 1:A:15:PHE:HD2  | 1:A:35:GLY:H     | 2        | 2.52          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2   | 1        | 2.51          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2   | 1        | 2.51          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2   | 1        | 2.51          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 16       | 2.51          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2   | 1        | 2.51          |
| (1,1783) | 1:A:17:PHE:H    | 1:A:33:TYR:HD2   | 3        | 2.51          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG21 | 19       | 2.51          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG22 | 19       | 2.51          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG23 | 19       | 2.51          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2   | 7        | 2.51          |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA2   | 12       | 2.5           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA3  | 12       | 2.5           |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 13       | 2.5           |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 9        | 2.5           |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 9        | 2.5           |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 9        | 2.5           |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 3        | 2.5           |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 13       | 2.5           |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 8        | 2.5           |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 8        | 2.5           |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 8        | 2.5           |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1  | 8        | 2.5           |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 1        | 2.5           |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2  | 6        | 2.49          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 4        | 2.49          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 8        | 2.49          |
| (1,1742) | 1:A:32:LEU:HD21 | 1:A:33:TYR:HD2  | 11       | 2.49          |
| (1,1742) | 1:A:32:LEU:HD22 | 1:A:33:TYR:HD2  | 11       | 2.49          |
| (1,1742) | 1:A:32:LEU:HD23 | 1:A:33:TYR:HD2  | 11       | 2.49          |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 10       | 2.49          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 19       | 2.48          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 19       | 2.48          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 19       | 2.48          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 3        | 2.48          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 3        | 2.48          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 3        | 2.48          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 11       | 2.48          |
| (1,470)  | 1:A:68:PHE:HE2  | 1:A:94:ILE:H    | 19       | 2.47          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2  | 8        | 2.47          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3  | 8        | 2.47          |
| (1,1776) | 1:A:15:PHE:HD1  | 1:A:110:THR:HB  | 4        | 2.47          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 3        | 2.47          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 3        | 2.47          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 3        | 2.47          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 20       | 2.46          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 7        | 2.46          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 16       | 2.45          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 12       | 2.45          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 5        | 2.45          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 10       | 2.45          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 16       | 2.45          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2  | 10       | 2.44          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3  | 10       | 2.44          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2  | 10       | 2.44          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3  | 10       | 2.44          |
| (1,1811) | 1:A:67:TYR:HD1  | 1:A:81:SER:H    | 15       | 2.44          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 19       | 2.44          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 17       | 2.44          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 17       | 2.44          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 17       | 2.44          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 16       | 2.43          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 16       | 2.43          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 11       | 2.43          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2  | 17       | 2.43          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 12       | 2.43          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 10       | 2.43          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 10       | 2.43          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 10       | 2.43          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2  | 5        | 2.42          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 8        | 2.42          |
| (1,1776) | 1:A:15:PHE:HD1  | 1:A:110:THR:HB  | 3        | 2.42          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 14       | 2.42          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 14       | 2.42          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 14       | 2.42          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 11       | 2.42          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 14       | 2.41          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 14       | 2.41          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 14       | 2.41          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2  | 11       | 2.41          |
| (1,1815) | 1:A:61:ALA:HA   | 1:A:67:TYR:HE2  | 14       | 2.41          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 3        | 2.41          |
| (1,1795) | 1:A:17:PHE:H    | 1:A:33:TYR:HE2  | 14       | 2.41          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 12       | 2.41          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1  | 20       | 2.41          |
| (1,1109) | 1:A:15:PHE:HD2  | 1:A:33:TYR:HB3  | 11       | 2.41          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 16       | 2.4           |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 16       | 2.4           |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 16       | 2.4           |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 5        | 2.4           |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 18       | 2.4           |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 13       | 2.4           |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 5        | 2.4           |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 9        | 2.4           |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 11       | 2.4           |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 5        | 2.4           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2200) | 1:A:68:PHE:HE2  | 1:A:93:GLY:HA2  | 17       | 2.39          |
| (1,2200) | 1:A:68:PHE:HE2  | 1:A:93:GLY:HA3  | 17       | 2.39          |
| (1,1806) | 1:A:61:ALA:H    | 1:A:67:TYR:HD2  | 14       | 2.39          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB1  | 20       | 2.38          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB2  | 20       | 2.38          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB3  | 20       | 2.38          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 2        | 2.38          |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 13       | 2.38          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 18       | 2.37          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2  | 4        | 2.37          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 10       | 2.37          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 10       | 2.37          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 10       | 2.37          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 14       | 2.37          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 9        | 2.37          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 13       | 2.37          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 13       | 2.37          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 13       | 2.37          |
| (1,774)  | 1:A:60:VAL:HG11 | 1:A:67:TYR:HD2  | 8        | 2.36          |
| (1,774)  | 1:A:60:VAL:HG12 | 1:A:67:TYR:HD2  | 8        | 2.36          |
| (1,774)  | 1:A:60:VAL:HG13 | 1:A:67:TYR:HD2  | 8        | 2.36          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2  | 8        | 2.36          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3  | 8        | 2.36          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 2        | 2.36          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 9        | 2.36          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 7        | 2.36          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 20       | 2.36          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 20       | 2.36          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 20       | 2.36          |
| (1,879)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1  | 10       | 2.35          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 17       | 2.35          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 17       | 2.35          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 17       | 2.35          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 15       | 2.35          |
| (1,470)  | 1:A:68:PHE:HE2  | 1:A:94:ILE:H    | 17       | 2.34          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 6        | 2.34          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 17       | 2.34          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 11       | 2.34          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 11       | 2.34          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 11       | 2.34          |
| (1,115)  | 1:A:15:PHE:HD2  | 1:A:35:GLY:H    | 20       | 2.34          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 13       | 2.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 8        | 2.33          |
| (1,1781) | 1:A:16:LYS:HB2  | 1:A:33:TYR:HD2  | 18       | 2.33          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 16       | 2.33          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 16       | 2.33          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 16       | 2.33          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 16       | 2.33          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 9        | 2.32          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 4        | 2.32          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 4        | 2.32          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 4        | 2.32          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 10       | 2.32          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 19       | 2.32          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 2        | 2.32          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 2        | 2.32          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 2        | 2.32          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 7        | 2.32          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 7        | 2.32          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 7        | 2.32          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 15       | 2.32          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 15       | 2.32          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 15       | 2.32          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 19       | 2.31          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 19       | 2.31          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 19       | 2.31          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 3        | 2.31          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 3        | 2.31          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 3        | 2.31          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 8        | 2.31          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 8        | 2.31          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 8        | 2.31          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 20       | 2.31          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 6        | 2.31          |
| (1,1109) | 1:A:15:PHE:HD2  | 1:A:33:TYR:HB3  | 19       | 2.31          |
| (1,2136) | 1:A:56:TYR:HB2  | 1:A:68:PHE:HD1  | 9        | 2.3           |
| (1,2136) | 1:A:56:TYR:HB3  | 1:A:68:PHE:HD1  | 9        | 2.3           |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 11       | 2.3           |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 11       | 2.3           |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 11       | 2.3           |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 20       | 2.3           |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 12       | 2.3           |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 13       | 2.3           |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 20       | 2.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 20       | 2.3           |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 20       | 2.3           |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2  | 3        | 2.29          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3  | 3        | 2.29          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 20       | 2.29          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 20       | 2.29          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 20       | 2.29          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 20       | 2.29          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 20       | 2.29          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 20       | 2.29          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 11       | 2.29          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 6        | 2.29          |
| (1,1780) | 1:A:15:PHE:HE1  | 1:A:110:THR:HB  | 10       | 2.29          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 13       | 2.29          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 8        | 2.29          |
| (1,859)  | 1:A:7:LEU:HG    | 1:A:15:PHE:HD1  | 20       | 2.28          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 5        | 2.28          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 5        | 2.28          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 5        | 2.28          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 2        | 2.28          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 19       | 2.28          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA2  | 12       | 2.27          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA3  | 12       | 2.27          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2  | 3        | 2.27          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2  | 3        | 2.27          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2  | 3        | 2.27          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 7        | 2.27          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 9        | 2.27          |
| (1,1792) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA2  | 6        | 2.27          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 8        | 2.27          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1  | 3        | 2.27          |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 12       | 2.27          |
| (1,1109) | 1:A:15:PHE:HD2  | 1:A:33:TYR:HB3  | 20       | 2.27          |
| (1,1776) | 1:A:15:PHE:HD1  | 1:A:110:THR:HB  | 11       | 2.26          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2  | 12       | 2.26          |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 9        | 2.26          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 5        | 2.25          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 19       | 2.25          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 9        | 2.25          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 9        | 2.25          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 9        | 2.25          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 1        | 2.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 1        | 2.25          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 1        | 2.25          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 18       | 2.25          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 18       | 2.25          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 18       | 2.25          |
| (1,1385) | 1:A:66:PRO:HB2  | 1:A:84:TYR:HD1  | 10       | 2.25          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 12       | 2.24          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 12       | 2.24          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2  | 17       | 2.24          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 19       | 2.24          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 15       | 2.24          |
| (1,879)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1  | 12       | 2.23          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 12       | 2.23          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2  | 6        | 2.23          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3  | 6        | 2.23          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1  | 20       | 2.23          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2  | 20       | 2.23          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3  | 20       | 2.23          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 11       | 2.23          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 12       | 2.23          |
| (1,1776) | 1:A:15:PHE:HD1  | 1:A:110:THR:HB  | 20       | 2.23          |
| (1,859)  | 1:A:7:LEU:HG    | 1:A:15:PHE:HD1  | 11       | 2.22          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2  | 2        | 2.22          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2  | 2        | 2.22          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 5        | 2.22          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 5        | 2.22          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 5        | 2.22          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2  | 10       | 2.22          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2  | 10       | 2.22          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2  | 10       | 2.22          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 13       | 2.22          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 5        | 2.22          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2  | 2        | 2.22          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2  | 4        | 2.22          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2  | 11       | 2.22          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2  | 3        | 2.22          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2  | 8        | 2.22          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2  | 16       | 2.22          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 5        | 2.22          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 5        | 2.22          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 5        | 2.22          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 10       | 2.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 10       | 2.22          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 10       | 2.22          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 13       | 2.22          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 13       | 2.22          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 13       | 2.22          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 6        | 2.22          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 6        | 2.22          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 6        | 2.22          |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 4        | 2.22          |
| (1,1109) | 1:A:15:PHE:HD2  | 1:A:33:TYR:HB3  | 6        | 2.22          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 18       | 2.21          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 18       | 2.21          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 18       | 2.21          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 12       | 2.21          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 14       | 2.2           |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2  | 4        | 2.2           |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3  | 4        | 2.2           |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2  | 7        | 2.2           |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3  | 7        | 2.2           |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 1        | 2.2           |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 2        | 2.2           |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 14       | 2.2           |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3  | 1        | 2.2           |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 1        | 2.2           |
| (1,1776) | 1:A:15:PHE:HD1  | 1:A:110:THR:HB  | 12       | 2.2           |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11 | 5        | 2.2           |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12 | 5        | 2.2           |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13 | 5        | 2.2           |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2  | 12       | 2.2           |
| (1,1109) | 1:A:15:PHE:HD2  | 1:A:33:TYR:HB3  | 15       | 2.2           |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 6        | 2.19          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 7        | 2.19          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 7        | 2.19          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 7        | 2.19          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 13       | 2.19          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 13       | 2.19          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 13       | 2.19          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2  | 10       | 2.19          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 2        | 2.19          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 2        | 2.19          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 2        | 2.19          |
| (1,2200) | 1:A:68:PHE:HE2  | 1:A:93:GLY:HA2  | 19       | 2.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2200) | 1:A:68:PHE:HE2  | 1:A:93:GLY:HA3  | 19       | 2.18          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 14       | 2.18          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 14       | 2.18          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 15       | 2.18          |
| (1,115)  | 1:A:15:PHE:HD2  | 1:A:35:GLY:H    | 7        | 2.18          |
| (1,1109) | 1:A:15:PHE:HD2  | 1:A:33:TYR:HB3  | 2        | 2.18          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 13       | 2.17          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2  | 15       | 2.17          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2  | 15       | 2.17          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2  | 15       | 2.17          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 16       | 2.17          |
| (1,859)  | 1:A:7:LEU:HG    | 1:A:15:PHE:HD1  | 15       | 2.16          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 6        | 2.16          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 6        | 2.16          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 6        | 2.16          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2  | 2        | 2.16          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2  | 2        | 2.16          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2  | 2        | 2.16          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 18       | 2.16          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2  | 3        | 2.16          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2  | 19       | 2.15          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2  | 19       | 2.15          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 6        | 2.15          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 6        | 2.15          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 6        | 2.15          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 8        | 2.15          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 17       | 2.15          |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 18       | 2.15          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 14       | 2.15          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 14       | 2.15          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 14       | 2.15          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 11       | 2.14          |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1  | 15       | 2.14          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2  | 19       | 2.14          |
| (1,1109) | 1:A:15:PHE:HD2  | 1:A:33:TYR:HB3  | 4        | 2.14          |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2  | 1        | 2.13          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 18       | 2.13          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 18       | 2.13          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 18       | 2.13          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 16       | 2.13          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 16       | 2.13          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 16       | 2.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 11       | 2.13          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21 | 8        | 2.13          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22 | 8        | 2.13          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23 | 8        | 2.13          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 8        | 2.13          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 8        | 2.13          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 8        | 2.13          |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 20       | 2.13          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 13       | 2.12          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 13       | 2.12          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2  | 18       | 2.12          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2  | 18       | 2.12          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2  | 18       | 2.12          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 3        | 2.12          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2  | 13       | 2.12          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1  | 18       | 2.12          |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1  | 3        | 2.11          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 15       | 2.11          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2  | 16       | 2.11          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 13       | 2.11          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 2        | 2.11          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 13       | 2.11          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2  | 7        | 2.11          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2  | 13       | 2.1           |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3  | 13       | 2.1           |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 19       | 2.1           |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 19       | 2.1           |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 19       | 2.1           |
| (1,1744) | 1:A:30:SER:HA   | 1:A:33:TYR:HE2  | 14       | 2.1           |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 6        | 2.1           |
| (1,1400) | 1:A:67:TYR:HA   | 1:A:84:TYR:HD1  | 7        | 2.1           |
| (1,1843) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1  | 3        | 2.09          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1  | 15       | 2.09          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 3        | 2.09          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 3        | 2.09          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 3        | 2.09          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 9        | 2.09          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 9        | 2.09          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 9        | 2.09          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2  | 12       | 2.09          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2  | 12       | 2.09          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2  | 12       | 2.09          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1800) | 1:A:33:TYR:HE1 | 1:A:38:GLY:HA3  | 8        | 2.09          |
| (1,1792) | 1:A:33:TYR:HD1 | 1:A:38:GLY:HA2  | 15       | 2.09          |
| (1,879)  | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 7        | 2.08          |
| (1,2259) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HG2  | 15       | 2.08          |
| (1,2259) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HG3  | 15       | 2.08          |
| (1,2031) | 1:A:30:SER:HB2 | 1:A:33:TYR:HD2  | 16       | 2.08          |
| (1,2031) | 1:A:30:SER:HB3 | 1:A:33:TYR:HD2  | 16       | 2.08          |
| (1,1821) | 1:A:61:ALA:H   | 1:A:67:TYR:HE2  | 8        | 2.08          |
| (1,1407) | 1:A:67:TYR:HB3 | 1:A:84:TYR:HD1  | 16       | 2.08          |
| (1,783)  | 1:A:30:SER:HB2 | 1:A:33:TYR:HE2  | 3        | 2.07          |
| (1,783)  | 1:A:30:SER:HB2 | 1:A:33:TYR:HE2  | 18       | 2.07          |
| (1,1816) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HE2  | 17       | 2.07          |
| (1,1816) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HE2  | 17       | 2.07          |
| (1,1816) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HE2  | 17       | 2.07          |
| (1,1805) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HD2  | 4        | 2.07          |
| (1,1805) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HD2  | 4        | 2.07          |
| (1,1805) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HD2  | 4        | 2.07          |
| (1,1805) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HD2  | 14       | 2.07          |
| (1,1805) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HD2  | 14       | 2.07          |
| (1,1805) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HD2  | 14       | 2.07          |
| (1,1805) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HD2  | 15       | 2.07          |
| (1,1805) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HD2  | 15       | 2.07          |
| (1,1805) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HD2  | 15       | 2.07          |
| (1,1802) | 1:A:30:SER:HB3 | 1:A:33:TYR:HE2  | 17       | 2.07          |
| (1,1796) | 1:A:31:GLU:H   | 1:A:33:TYR:HE2  | 20       | 2.07          |
| (1,1791) | 1:A:33:TYR:HD1 | 1:A:38:GLY:HA3  | 6        | 2.07          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG21 | 15       | 2.07          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG22 | 15       | 2.07          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG23 | 15       | 2.07          |
| (1,783)  | 1:A:30:SER:HB2 | 1:A:33:TYR:HE2  | 9        | 2.06          |
| (1,2030) | 1:A:30:SER:HB2 | 1:A:33:TYR:HE2  | 6        | 2.06          |
| (1,2030) | 1:A:30:SER:HB3 | 1:A:33:TYR:HE2  | 6        | 2.06          |
| (1,1741) | 1:A:61:ALA:HA  | 1:A:67:TYR:HD2  | 18       | 2.06          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG21 | 12       | 2.06          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG22 | 12       | 2.06          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG23 | 12       | 2.06          |
| (1,1423) | 1:A:68:PHE:HE1 | 1:A:70:LEU:HD11 | 10       | 2.06          |
| (1,1423) | 1:A:68:PHE:HE1 | 1:A:70:LEU:HD12 | 10       | 2.06          |
| (1,1423) | 1:A:68:PHE:HE1 | 1:A:70:LEU:HD13 | 10       | 2.06          |
| (1,1132) | 1:A:33:TYR:HE1 | 1:A:38:GLY:HA2  | 6        | 2.06          |
| (1,859)  | 1:A:7:LEU:HG   | 1:A:15:PHE:HD1  | 4        | 2.05          |
| (1,1816) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HE2  | 20       | 2.05          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2   | 20       | 2.05          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2   | 20       | 2.05          |
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H     | 4        | 2.05          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1   | 3        | 2.05          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 20       | 2.04          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 4        | 2.04          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 4        | 2.04          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 4        | 2.04          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2   | 15       | 2.04          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2   | 15       | 2.04          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2   | 15       | 2.04          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 7        | 2.04          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 7        | 2.04          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 7        | 2.04          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3   | 19       | 2.03          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3   | 20       | 2.03          |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1   | 17       | 2.03          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11  | 4        | 2.03          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12  | 4        | 2.03          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13  | 4        | 2.03          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1   | 1        | 2.03          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2   | 8        | 2.02          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3   | 8        | 2.02          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2   | 14       | 2.02          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2   | 16       | 2.02          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11  | 13       | 2.02          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12  | 13       | 2.02          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13  | 13       | 2.02          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2   | 18       | 2.01          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3   | 18       | 2.01          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 11       | 2.01          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 11       | 2.01          |
| (1,1780) | 1:A:15:PHE:HE1  | 1:A:110:THR:HB   | 2        | 2.01          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1   | 12       | 2.01          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2   | 11       | 2.0           |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3   | 11       | 2.0           |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 1        | 2.0           |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 1        | 2.0           |
| (1,1821) | 1:A:61:ALA:H    | 1:A:67:TYR:HE2   | 14       | 2.0           |
| (1,1776) | 1:A:15:PHE:HD1  | 1:A:110:THR:HB   | 7        | 2.0           |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H     | 10       | 2.0           |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 6        | 1.99          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2  | 6        | 1.99          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2  | 6        | 1.99          |
| (1,2245) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1  | 3        | 1.99          |
| (1,2245) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1  | 3        | 1.99          |
| (1,1843) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1  | 20       | 1.99          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 17       | 1.99          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 17       | 1.99          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 17       | 1.99          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2  | 1        | 1.99          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2  | 1        | 1.99          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2  | 1        | 1.99          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2  | 9        | 1.99          |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H    | 13       | 1.99          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2  | 4        | 1.99          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 20       | 1.99          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 20       | 1.99          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 20       | 1.99          |
| (1,2136) | 1:A:56:TYR:HB2  | 1:A:68:PHE:HD1  | 7        | 1.98          |
| (1,2136) | 1:A:56:TYR:HB3  | 1:A:68:PHE:HD1  | 7        | 1.98          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 9        | 1.98          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 9        | 1.98          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 18       | 1.98          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2  | 18       | 1.98          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2  | 12       | 1.98          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2  | 12       | 1.98          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2  | 12       | 1.98          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3  | 12       | 1.98          |
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H    | 3        | 1.98          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 15       | 1.97          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2  | 1        | 1.97          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3  | 1        | 1.97          |
| (1,2136) | 1:A:56:TYR:HB2  | 1:A:68:PHE:HD1  | 6        | 1.97          |
| (1,2136) | 1:A:56:TYR:HB3  | 1:A:68:PHE:HD1  | 6        | 1.97          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2  | 9        | 1.97          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2  | 9        | 1.97          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2  | 9        | 1.97          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2  | 12       | 1.97          |
| (1,1780) | 1:A:15:PHE:HE1  | 1:A:110:THR:HB  | 6        | 1.97          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1  | 11       | 1.97          |
| (1,1109) | 1:A:15:PHE:HD2  | 1:A:33:TYR:HB3  | 10       | 1.97          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2  | 11       | 1.96          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3  | 11       | 1.96          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1813) | 1:A:60:VAL:H   | 1:A:67:TYR:HE2  | 6        | 1.96          |
| (1,1776) | 1:A:15:PHE:HD1 | 1:A:110:THR:HB  | 15       | 1.96          |
| (1,1741) | 1:A:61:ALA:HA  | 1:A:67:TYR:HD2  | 14       | 1.96          |
| (1,1406) | 1:A:67:TYR:HB2 | 1:A:84:TYR:HD1  | 14       | 1.96          |
| (1,1385) | 1:A:66:PRO:HB2 | 1:A:84:TYR:HD1  | 16       | 1.96          |
| (1,1820) | 1:A:67:TYR:HE1 | 1:A:80:THR:HG21 | 16       | 1.95          |
| (1,1820) | 1:A:67:TYR:HE1 | 1:A:80:THR:HG22 | 16       | 1.95          |
| (1,1820) | 1:A:67:TYR:HE1 | 1:A:80:THR:HG23 | 16       | 1.95          |
| (1,1813) | 1:A:60:VAL:H   | 1:A:67:TYR:HE2  | 19       | 1.95          |
| (1,1802) | 1:A:30:SER:HB3 | 1:A:33:TYR:HE2  | 6        | 1.95          |
| (1,1109) | 1:A:15:PHE:HD2 | 1:A:33:TYR:HB3  | 5        | 1.95          |
| (1,2031) | 1:A:30:SER:HB2 | 1:A:33:TYR:HD2  | 12       | 1.94          |
| (1,2031) | 1:A:30:SER:HB3 | 1:A:33:TYR:HD2  | 12       | 1.94          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB1  | 14       | 1.94          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB2  | 14       | 1.94          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB3  | 14       | 1.94          |
| (1,1814) | 1:A:60:VAL:HA  | 1:A:67:TYR:HE2  | 12       | 1.94          |
| (1,1782) | 1:A:16:LYS:HB3 | 1:A:33:TYR:HD2  | 3        | 1.94          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG21 | 4        | 1.94          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG22 | 4        | 1.94          |
| (1,1518) | 1:A:67:TYR:HD1 | 1:A:80:THR:HG23 | 4        | 1.94          |
| (1,852)  | 1:A:7:LEU:HD21 | 1:A:15:PHE:HD1  | 11       | 1.93          |
| (1,852)  | 1:A:7:LEU:HD22 | 1:A:15:PHE:HD1  | 11       | 1.93          |
| (1,852)  | 1:A:7:LEU:HD23 | 1:A:15:PHE:HD1  | 11       | 1.93          |
| (1,2030) | 1:A:30:SER:HB2 | 1:A:33:TYR:HE2  | 20       | 1.93          |
| (1,2030) | 1:A:30:SER:HB3 | 1:A:33:TYR:HE2  | 20       | 1.93          |
| (1,1821) | 1:A:61:ALA:H   | 1:A:67:TYR:HE2  | 12       | 1.93          |
| (1,1816) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HE2  | 4        | 1.93          |
| (1,1816) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HE2  | 4        | 1.93          |
| (1,1816) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HE2  | 4        | 1.93          |
| (1,1816) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HE2  | 5        | 1.93          |
| (1,1816) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HE2  | 5        | 1.93          |
| (1,1816) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HE2  | 5        | 1.93          |
| (1,1816) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HE2  | 16       | 1.93          |
| (1,1816) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HE2  | 16       | 1.93          |
| (1,1816) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HE2  | 16       | 1.93          |
| (1,1743) | 1:A:33:TYR:HD1 | 1:A:35:GLY:H    | 9        | 1.93          |
| (1,1132) | 1:A:33:TYR:HE1 | 1:A:38:GLY:HA2  | 1        | 1.93          |
| (1,2260) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HG2  | 15       | 1.92          |
| (1,2260) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HG3  | 15       | 1.92          |
| (1,1965) | 1:A:15:PHE:HD2 | 1:A:35:GLY:HA2  | 5        | 1.92          |
| (1,1965) | 1:A:15:PHE:HD2 | 1:A:35:GLY:HA3  | 5        | 1.92          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA2   | 5        | 1.92          |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA3   | 5        | 1.92          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB1   | 9        | 1.92          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB2   | 9        | 1.92          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB3   | 9        | 1.92          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2   | 8        | 1.92          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2   | 8        | 1.92          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2   | 8        | 1.92          |
| (1,1780) | 1:A:15:PHE:HE1  | 1:A:110:THR:HB   | 5        | 1.92          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11  | 1        | 1.92          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12  | 1        | 1.92          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13  | 1        | 1.92          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11  | 15       | 1.92          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12  | 15       | 1.92          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13  | 15       | 1.92          |
| (1,1109) | 1:A:15:PHE:HD2  | 1:A:33:TYR:HB3   | 3        | 1.92          |
| (1,1804) | 1:A:60:VAL:HA   | 1:A:67:TYR:HD2   | 8        | 1.91          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 9        | 1.91          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 20       | 1.91          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 20       | 1.91          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 20       | 1.91          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11  | 12       | 1.91          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12  | 12       | 1.91          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13  | 12       | 1.91          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 7        | 1.91          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 10       | 1.9           |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 10       | 1.9           |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 10       | 1.9           |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2   | 13       | 1.9           |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 18       | 1.9           |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2   | 5        | 1.9           |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1   | 5        | 1.9           |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 12       | 1.9           |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 12       | 1.9           |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 12       | 1.9           |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 15       | 1.9           |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 15       | 1.9           |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 15       | 1.9           |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21  | 9        | 1.9           |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22  | 9        | 1.9           |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23  | 9        | 1.9           |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11  | 18       | 1.9           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12  | 18       | 1.9           |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13  | 18       | 1.9           |
| (1,852)  | 1:A:7:LEU:HD21  | 1:A:15:PHE:HD1   | 15       | 1.89          |
| (1,852)  | 1:A:7:LEU:HD22  | 1:A:15:PHE:HD1   | 15       | 1.89          |
| (1,852)  | 1:A:7:LEU:HD23  | 1:A:15:PHE:HD1   | 15       | 1.89          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 7        | 1.89          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 7        | 1.89          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 7        | 1.89          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 3        | 1.89          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 3        | 1.89          |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA2   | 7        | 1.89          |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA3   | 7        | 1.89          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1   | 3        | 1.89          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21  | 5        | 1.89          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22  | 5        | 1.89          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23  | 5        | 1.89          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 11       | 1.89          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2   | 12       | 1.89          |
| (1,877)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1   | 10       | 1.88          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2   | 2        | 1.88          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2   | 2        | 1.88          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2   | 2        | 1.88          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2   | 7        | 1.88          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 9        | 1.88          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 13       | 1.88          |
| (1,859)  | 1:A:7:LEU:HG    | 1:A:15:PHE:HD1   | 7        | 1.87          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 4        | 1.87          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 4        | 1.87          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 7        | 1.87          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 7        | 1.87          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2   | 11       | 1.87          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2   | 11       | 1.87          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2   | 11       | 1.87          |
| (1,1805) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HD2   | 13       | 1.87          |
| (1,1805) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HD2   | 13       | 1.87          |
| (1,1805) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HD2   | 13       | 1.87          |
| (1,1791) | 1:A:33:TYR:HD1  | 1:A:38:GLY:HA3   | 15       | 1.87          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 11       | 1.87          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 11       | 1.87          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 11       | 1.87          |
| (1,1385) | 1:A:66:PRO:HB2  | 1:A:84:TYR:HD1   | 8        | 1.87          |
| (1,859)  | 1:A:7:LEU:HG    | 1:A:15:PHE:HD1   | 6        | 1.86          |

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| Key      | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,2245) | 1:A:81:SER:HB2 | 1:A:84:TYR:HE1 | 8        | 1.86          |
| (1,2245) | 1:A:81:SER:HB3 | 1:A:84:TYR:HE1 | 8        | 1.86          |
| (1,2031) | 1:A:30:SER:HB2 | 1:A:33:TYR:HD2 | 14       | 1.86          |
| (1,2031) | 1:A:30:SER:HB3 | 1:A:33:TYR:HD2 | 14       | 1.86          |
| (1,1843) | 1:A:81:SER:HB2 | 1:A:84:TYR:HE1 | 12       | 1.86          |
| (1,1811) | 1:A:67:TYR:HD1 | 1:A:81:SER:H   | 20       | 1.86          |
| (1,1805) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HD2 | 11       | 1.86          |
| (1,1805) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HD2 | 11       | 1.86          |
| (1,1805) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HD2 | 11       | 1.86          |
| (1,1782) | 1:A:16:LYS:HB3 | 1:A:33:TYR:HD2 | 14       | 1.86          |
| (1,1523) | 1:A:81:SER:HA  | 1:A:84:TYR:HE1 | 15       | 1.86          |
| (1,1407) | 1:A:67:TYR:HB3 | 1:A:84:TYR:HD1 | 3        | 1.86          |
| (1,1383) | 1:A:66:PRO:HA  | 1:A:67:TYR:HD2 | 17       | 1.86          |
| (1,859)  | 1:A:7:LEU:HG   | 1:A:15:PHE:HD1 | 19       | 1.85          |
| (1,1805) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HD2 | 6        | 1.85          |
| (1,1805) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HD2 | 6        | 1.85          |
| (1,1805) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HD2 | 6        | 1.85          |
| (1,1743) | 1:A:33:TYR:HD1 | 1:A:35:GLY:H   | 17       | 1.85          |
| (1,1383) | 1:A:66:PRO:HA  | 1:A:67:TYR:HD2 | 4        | 1.85          |
| (1,1109) | 1:A:15:PHE:HD2 | 1:A:33:TYR:HB3 | 7        | 1.85          |
| (1,1814) | 1:A:60:VAL:HA  | 1:A:67:TYR:HE2 | 11       | 1.84          |
| (1,1813) | 1:A:60:VAL:H   | 1:A:67:TYR:HE2 | 20       | 1.84          |
| (1,1805) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HD2 | 7        | 1.84          |
| (1,1805) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HD2 | 7        | 1.84          |
| (1,1805) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HD2 | 7        | 1.84          |
| (1,1800) | 1:A:33:TYR:HE1 | 1:A:38:GLY:HA3 | 6        | 1.84          |
| (1,1796) | 1:A:31:GLU:H   | 1:A:33:TYR:HE2 | 8        | 1.84          |
| (1,1383) | 1:A:66:PRO:HA  | 1:A:67:TYR:HD2 | 5        | 1.84          |
| (1,1383) | 1:A:66:PRO:HA  | 1:A:67:TYR:HD2 | 6        | 1.84          |
| (1,852)  | 1:A:7:LEU:HD21 | 1:A:15:PHE:HD1 | 20       | 1.83          |
| (1,852)  | 1:A:7:LEU:HD22 | 1:A:15:PHE:HD1 | 20       | 1.83          |
| (1,852)  | 1:A:7:LEU:HD23 | 1:A:15:PHE:HD1 | 20       | 1.83          |
| (1,2259) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HG2 | 12       | 1.83          |
| (1,2259) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HG3 | 12       | 1.83          |
| (1,1816) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HE2 | 7        | 1.83          |
| (1,1816) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HE2 | 7        | 1.83          |
| (1,1816) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HE2 | 7        | 1.83          |
| (1,1780) | 1:A:15:PHE:HE1 | 1:A:110:THR:HB | 19       | 1.83          |
| (1,1743) | 1:A:33:TYR:HD1 | 1:A:35:GLY:H   | 3        | 1.83          |
| (1,1741) | 1:A:61:ALA:HA  | 1:A:67:TYR:HD2 | 2        | 1.83          |
| (1,877)  | 1:A:9:LYS:HB3  | 1:A:15:PHE:HD1 | 12       | 1.82          |
| (1,2031) | 1:A:30:SER:HB2 | 1:A:33:TYR:HD2 | 13       | 1.82          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2   | 13       | 1.82          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1   | 9        | 1.82          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2   | 9        | 1.82          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3   | 9        | 1.82          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2   | 1        | 1.82          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2   | 1        | 1.82          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2   | 1        | 1.82          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2   | 11       | 1.82          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2   | 11       | 1.82          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2   | 11       | 1.82          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2   | 7        | 1.82          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 20       | 1.82          |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1   | 14       | 1.82          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1   | 14       | 1.82          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11  | 16       | 1.82          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12  | 16       | 1.82          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13  | 16       | 1.82          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2   | 2        | 1.81          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2   | 3        | 1.81          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA2   | 7        | 1.8           |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA3   | 7        | 1.8           |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2   | 6        | 1.8           |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2   | 6        | 1.8           |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2   | 6        | 1.8           |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2   | 2        | 1.8           |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1   | 15       | 1.8           |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1   | 10       | 1.79          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 5        | 1.79          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 5        | 1.79          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 5        | 1.79          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11  | 7        | 1.79          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12  | 7        | 1.79          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13  | 7        | 1.79          |
| (1,2245) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1   | 20       | 1.78          |
| (1,2245) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1   | 20       | 1.78          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2   | 16       | 1.78          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2   | 16       | 1.78          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2   | 16       | 1.78          |
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H     | 1        | 1.78          |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1   | 4        | 1.78          |
| (1,887)  | 1:A:9:LYS:HG2   | 1:A:15:PHE:HE1   | 10       | 1.77          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2   | 16       | 1.77          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3   | 16       | 1.77          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 15       | 1.77          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 15       | 1.77          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21  | 8        | 1.77          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22  | 8        | 1.77          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23  | 8        | 1.77          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2   | 15       | 1.77          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 13       | 1.76          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 13       | 1.76          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 13       | 1.76          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2   | 11       | 1.76          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2   | 11       | 1.76          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA2   | 10       | 1.76          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA3   | 10       | 1.76          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2   | 14       | 1.76          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2   | 14       | 1.76          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2   | 14       | 1.76          |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2   | 6        | 1.76          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 12       | 1.76          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 15       | 1.76          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 18       | 1.75          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 18       | 1.75          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 18       | 1.75          |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1   | 20       | 1.75          |
| (1,1780) | 1:A:15:PHE:HE1  | 1:A:110:THR:HB   | 12       | 1.75          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21  | 2        | 1.75          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22  | 2        | 1.75          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23  | 2        | 1.75          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 19       | 1.75          |
| (1,1132) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA2   | 15       | 1.75          |
| (1,859)  | 1:A:7:LEU:HG    | 1:A:15:PHE:HD1   | 3        | 1.74          |
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H     | 14       | 1.74          |
| (1,1780) | 1:A:15:PHE:HE1  | 1:A:110:THR:HB   | 3        | 1.73          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 4        | 1.73          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 4        | 1.73          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 4        | 1.73          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2   | 6        | 1.72          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3   | 6        | 1.72          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21  | 13       | 1.72          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22  | 13       | 1.72          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23  | 13       | 1.72          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 6        | 1.72          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 6        | 1.72          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 6        | 1.72          |
| (1,117)  | 1:A:15:PHE:HE2  | 1:A:36:LYS:H     | 12       | 1.72          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 5        | 1.71          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 5        | 1.71          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2   | 16       | 1.71          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 3        | 1.71          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1   | 13       | 1.71          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 20       | 1.71          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2   | 15       | 1.7           |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3   | 15       | 1.7           |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2   | 6        | 1.7           |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2   | 6        | 1.7           |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA2   | 2        | 1.7           |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA3   | 2        | 1.7           |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA2   | 6        | 1.7           |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA3   | 6        | 1.7           |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB1   | 12       | 1.7           |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB2   | 12       | 1.7           |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB3   | 12       | 1.7           |
| (1,1780) | 1:A:15:PHE:HE1  | 1:A:110:THR:HB   | 7        | 1.7           |
| (1,1780) | 1:A:15:PHE:HE1  | 1:A:110:THR:HB   | 20       | 1.7           |
| (1,1741) | 1:A:61:ALA:HA   | 1:A:67:TYR:HD2   | 11       | 1.7           |
| (1,1407) | 1:A:67:TYR:HB3  | 1:A:84:TYR:HD1   | 18       | 1.7           |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1   | 20       | 1.7           |
| (1,859)  | 1:A:7:LEU:HG    | 1:A:15:PHE:HD1   | 12       | 1.69          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 3        | 1.69          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 3        | 1.69          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 3        | 1.69          |
| (1,2136) | 1:A:56:TYR:HB2  | 1:A:68:PHE:HD1   | 2        | 1.69          |
| (1,2136) | 1:A:56:TYR:HB3  | 1:A:68:PHE:HD1   | 2        | 1.69          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21  | 10       | 1.69          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22  | 10       | 1.69          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23  | 10       | 1.69          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2   | 3        | 1.68          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3   | 3        | 1.68          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1   | 11       | 1.68          |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2   | 1        | 1.68          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 2        | 1.68          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 2        | 1.68          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 2        | 1.68          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11  | 5        | 1.68          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12  | 5        | 1.68          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13  | 5        | 1.68          |
| (1,1407) | 1:A:67:TYR:HB3  | 1:A:84:TYR:HD1   | 8        | 1.68          |
| (1,859)  | 1:A:7:LEU:HG    | 1:A:15:PHE:HD1   | 5        | 1.67          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 10       | 1.67          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 10       | 1.67          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1   | 12       | 1.67          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2   | 12       | 1.67          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3   | 12       | 1.67          |
| (1,1780) | 1:A:15:PHE:HE1  | 1:A:110:THR:HB   | 4        | 1.67          |
| (1,859)  | 1:A:7:LEU:HG    | 1:A:15:PHE:HD1   | 10       | 1.66          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA2   | 6        | 1.66          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA3   | 6        | 1.66          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1   | 14       | 1.66          |
| (1,1780) | 1:A:15:PHE:HE1  | 1:A:110:THR:HB   | 11       | 1.66          |
| (1,1180) | 1:A:5:TYR:HD2   | 1:A:43:ILE:HG13  | 19       | 1.66          |
| (1,859)  | 1:A:7:LEU:HG    | 1:A:15:PHE:HD1   | 2        | 1.65          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1   | 14       | 1.65          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2   | 14       | 1.65          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3   | 14       | 1.65          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1   | 12       | 1.65          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2   | 9        | 1.65          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 19       | 1.65          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 19       | 1.65          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 19       | 1.65          |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA2   | 11       | 1.64          |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA3   | 11       | 1.64          |
| (1,1843) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1   | 14       | 1.64          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA    | 20       | 1.64          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1   | 1        | 1.64          |
| (1,1407) | 1:A:67:TYR:HB3  | 1:A:84:TYR:HD1   | 15       | 1.64          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 5        | 1.63          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 5        | 1.63          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 5        | 1.63          |
| (1,26)   | 1:A:6:GLU:H     | 1:A:17:PHE:HD1   | 4        | 1.63          |
| (1,2199) | 1:A:68:PHE:HE2  | 1:A:81:SER:HB2   | 19       | 1.63          |
| (1,2199) | 1:A:68:PHE:HE2  | 1:A:81:SER:HB3   | 19       | 1.63          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1   | 1        | 1.63          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2   | 1        | 1.63          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3   | 1        | 1.63          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 3        | 1.63          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 20       | 1.62          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 20       | 1.62          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 20       | 1.62          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2   | 3        | 1.62          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2   | 3        | 1.62          |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA2   | 20       | 1.62          |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA3   | 20       | 1.62          |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1   | 1        | 1.62          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB1   | 15       | 1.62          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB2   | 15       | 1.62          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB3   | 15       | 1.62          |
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H     | 18       | 1.62          |
| (1,1739) | 1:A:7:LEU:HD21  | 1:A:15:PHE:HE1   | 15       | 1.62          |
| (1,1739) | 1:A:7:LEU:HD22  | 1:A:15:PHE:HE1   | 15       | 1.62          |
| (1,1739) | 1:A:7:LEU:HD23  | 1:A:15:PHE:HE1   | 15       | 1.62          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 10       | 1.62          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 10       | 1.62          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 10       | 1.62          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG21 | 6        | 1.62          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG22 | 6        | 1.62          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG23 | 6        | 1.62          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2   | 9        | 1.61          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2   | 9        | 1.61          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2   | 20       | 1.61          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2   | 20       | 1.61          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB1   | 16       | 1.61          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB2   | 16       | 1.61          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB3   | 16       | 1.61          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2   | 14       | 1.61          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2   | 14       | 1.61          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2   | 14       | 1.61          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1   | 13       | 1.61          |
| (1,928)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:HA    | 6        | 1.6           |
| (1,877)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1   | 7        | 1.6           |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 11       | 1.6           |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 11       | 1.6           |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 11       | 1.6           |
| (1,26)   | 1:A:6:GLU:H     | 1:A:17:PHE:HD1   | 11       | 1.6           |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1   | 14       | 1.6           |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2   | 9        | 1.6           |
| (1,1407) | 1:A:67:TYR:HB3  | 1:A:84:TYR:HD1   | 11       | 1.6           |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 10       | 1.6           |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 17       | 1.59          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 17       | 1.59          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 17       | 1.59          |
| (1,26)   | 1:A:6:GLU:H     | 1:A:17:PHE:HD1   | 20       | 1.59          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2   | 18       | 1.59          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2   | 18       | 1.59          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 8        | 1.59          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 8        | 1.59          |
| (1,1823) | 1:A:68:PHE:HE2  | 1:A:81:SER:HB3   | 19       | 1.59          |
| (1,1816) | 1:A:61:ALA:HB1  | 1:A:67:TYR:HE2   | 13       | 1.59          |
| (1,1816) | 1:A:61:ALA:HB2  | 1:A:67:TYR:HE2   | 13       | 1.59          |
| (1,1816) | 1:A:61:ALA:HB3  | 1:A:67:TYR:HE2   | 13       | 1.59          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG21 | 3        | 1.59          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG22 | 3        | 1.59          |
| (1,1721) | 1:A:15:PHE:HE1  | 1:A:110:THR:HG23 | 3        | 1.59          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1   | 6        | 1.59          |
| (1,1398) | 1:A:66:PRO:HG2  | 1:A:84:TYR:HD1   | 10       | 1.59          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 16       | 1.59          |
| (1,928)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:HA    | 8        | 1.58          |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA2   | 4        | 1.58          |
| (1,1963) | 1:A:15:PHE:HE2  | 1:A:35:GLY:HA3   | 4        | 1.58          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1   | 15       | 1.58          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2   | 15       | 1.58          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3   | 15       | 1.58          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21  | 12       | 1.58          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22  | 12       | 1.58          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23  | 12       | 1.58          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2   | 19       | 1.58          |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1   | 8        | 1.58          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG21 | 11       | 1.58          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG22 | 11       | 1.58          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG23 | 11       | 1.58          |
| (1,2245) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1   | 14       | 1.57          |
| (1,2245) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1   | 14       | 1.57          |
| (1,2136) | 1:A:56:TYR:HB2  | 1:A:68:PHE:HD1   | 20       | 1.57          |
| (1,2136) | 1:A:56:TYR:HB3  | 1:A:68:PHE:HD1   | 20       | 1.57          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 1        | 1.57          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H     | 4        | 1.57          |
| (1,1780) | 1:A:15:PHE:HE1  | 1:A:110:THR:HB   | 15       | 1.57          |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H     | 8        | 1.57          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 8        | 1.57          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 18       | 1.57          |
| (1,928)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:HA    | 1        | 1.56          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,928)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:HA    | 2        | 1.56          |
| (1,928)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:HA    | 7        | 1.56          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 19       | 1.56          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 19       | 1.56          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 19       | 1.56          |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1   | 6        | 1.56          |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1   | 13       | 1.56          |
| (1,1818) | 1:A:60:VAL:HG11 | 1:A:67:TYR:HE2   | 8        | 1.56          |
| (1,1818) | 1:A:60:VAL:HG12 | 1:A:67:TYR:HE2   | 8        | 1.56          |
| (1,1818) | 1:A:60:VAL:HG13 | 1:A:67:TYR:HE2   | 8        | 1.56          |
| (1,1800) | 1:A:33:TYR:HE1  | 1:A:38:GLY:HA3   | 1        | 1.56          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG21 | 4        | 1.56          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG22 | 4        | 1.56          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG23 | 4        | 1.56          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1   | 12       | 1.56          |
| (1,1385) | 1:A:66:PRO:HB2  | 1:A:84:TYR:HD1   | 11       | 1.56          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 15       | 1.55          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 15       | 1.55          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 15       | 1.55          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2   | 6        | 1.55          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3   | 6        | 1.55          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2   | 4        | 1.55          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3   | 4        | 1.55          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2   | 15       | 1.55          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2   | 15       | 1.55          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 15       | 1.55          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2   | 10       | 1.55          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 11       | 1.55          |
| (1,928)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:HA    | 16       | 1.54          |
| (1,1884) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HB2   | 16       | 1.54          |
| (1,1884) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HB3   | 16       | 1.54          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1   | 16       | 1.54          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2   | 16       | 1.54          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3   | 16       | 1.54          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1   | 18       | 1.54          |
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H     | 17       | 1.54          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2   | 16       | 1.54          |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 1        | 1.54          |
| (1,928)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:HA    | 4        | 1.53          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA2   | 2        | 1.53          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA3   | 2        | 1.53          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1   | 1        | 1.53          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG21 | 20       | 1.53          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG22 | 20       | 1.53          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG23 | 20       | 1.53          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1   | 11       | 1.53          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG21  | 20       | 1.53          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG22  | 20       | 1.53          |
| (1,1518) | 1:A:67:TYR:HD1  | 1:A:80:THR:HG23  | 20       | 1.53          |
| (1,928)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:HA    | 18       | 1.52          |
| (1,928)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:HA    | 20       | 1.52          |
| (1,879)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1   | 20       | 1.52          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11  | 4        | 1.52          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12  | 4        | 1.52          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13  | 4        | 1.52          |
| (1,1385) | 1:A:66:PRO:HB2  | 1:A:84:TYR:HD1   | 4        | 1.52          |
| (1,1385) | 1:A:66:PRO:HB2  | 1:A:84:TYR:HD1   | 15       | 1.52          |
| (1,928)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:HA    | 11       | 1.51          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 12       | 1.51          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 12       | 1.51          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 12       | 1.51          |
| (1,2245) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1   | 12       | 1.51          |
| (1,2245) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1   | 12       | 1.51          |
| (1,2136) | 1:A:56:TYR:HB2  | 1:A:68:PHE:HD1   | 10       | 1.51          |
| (1,2136) | 1:A:56:TYR:HB3  | 1:A:68:PHE:HD1   | 10       | 1.51          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1   | 4        | 1.51          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2   | 4        | 1.51          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3   | 4        | 1.51          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2   | 4        | 1.51          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2   | 4        | 1.51          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2   | 4        | 1.51          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2   | 16       | 1.51          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG21 | 5        | 1.51          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG22 | 5        | 1.51          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG23 | 5        | 1.51          |
| (1,1385) | 1:A:66:PRO:HB2  | 1:A:84:TYR:HD1   | 14       | 1.51          |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG2   | 14       | 1.5           |
| (1,2259) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HG3   | 14       | 1.5           |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1   | 9        | 1.5           |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1   | 20       | 1.5           |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 2        | 1.5           |
| (1,1383) | 1:A:66:PRO:HA   | 1:A:67:TYR:HD2   | 14       | 1.5           |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2   | 7        | 1.49          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3   | 7        | 1.49          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1800) | 1:A:33:TYR:HE1 | 1:A:38:GLY:HA3   | 15       | 1.49          |
| (1,1784) | 1:A:33:TYR:H   | 1:A:33:TYR:HD2   | 3        | 1.49          |
| (1,1523) | 1:A:81:SER:HA  | 1:A:84:TYR:HE1   | 9        | 1.49          |
| (1,1407) | 1:A:67:TYR:HB3 | 1:A:84:TYR:HD1   | 1        | 1.49          |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD2   | 13       | 1.48          |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD3   | 13       | 1.48          |
| (1,1963) | 1:A:15:PHE:HE2 | 1:A:35:GLY:HA2   | 15       | 1.48          |
| (1,1963) | 1:A:15:PHE:HE2 | 1:A:35:GLY:HA3   | 15       | 1.48          |
| (1,1884) | 1:A:5:TYR:HD2  | 1:A:17:PHE:HB2   | 5        | 1.48          |
| (1,1884) | 1:A:5:TYR:HD2  | 1:A:17:PHE:HB3   | 5        | 1.48          |
| (1,1884) | 1:A:5:TYR:HD2  | 1:A:17:PHE:HB2   | 17       | 1.48          |
| (1,1884) | 1:A:5:TYR:HD2  | 1:A:17:PHE:HB3   | 17       | 1.48          |
| (1,1820) | 1:A:67:TYR:HE1 | 1:A:80:THR:HG21  | 15       | 1.48          |
| (1,1820) | 1:A:67:TYR:HE1 | 1:A:80:THR:HG22  | 15       | 1.48          |
| (1,1820) | 1:A:67:TYR:HE1 | 1:A:80:THR:HG23  | 15       | 1.48          |
| (1,1816) | 1:A:61:ALA:HB1 | 1:A:67:TYR:HE2   | 12       | 1.48          |
| (1,1816) | 1:A:61:ALA:HB2 | 1:A:67:TYR:HE2   | 12       | 1.48          |
| (1,1816) | 1:A:61:ALA:HB3 | 1:A:67:TYR:HE2   | 12       | 1.48          |
| (1,1814) | 1:A:60:VAL:HA  | 1:A:67:TYR:HE2   | 14       | 1.48          |
| (1,1798) | 1:A:33:TYR:HE1 | 1:A:42:GLY:H     | 9        | 1.48          |
| (1,2245) | 1:A:81:SER:HB2 | 1:A:84:TYR:HE1   | 1        | 1.47          |
| (1,2245) | 1:A:81:SER:HB3 | 1:A:84:TYR:HE1   | 1        | 1.47          |
| (1,2245) | 1:A:81:SER:HB2 | 1:A:84:TYR:HE1   | 13       | 1.47          |
| (1,2245) | 1:A:81:SER:HB3 | 1:A:84:TYR:HE1   | 13       | 1.47          |
| (1,1963) | 1:A:15:PHE:HE2 | 1:A:35:GLY:HA2   | 10       | 1.47          |
| (1,1963) | 1:A:15:PHE:HE2 | 1:A:35:GLY:HA3   | 10       | 1.47          |
| (1,1884) | 1:A:5:TYR:HD2  | 1:A:17:PHE:HB2   | 19       | 1.47          |
| (1,1884) | 1:A:5:TYR:HD2  | 1:A:17:PHE:HB3   | 19       | 1.47          |
| (1,1796) | 1:A:31:GLU:H   | 1:A:33:TYR:HE2   | 13       | 1.47          |
| (1,1739) | 1:A:7:LEU:HD21 | 1:A:15:PHE:HE1   | 20       | 1.47          |
| (1,1739) | 1:A:7:LEU:HD22 | 1:A:15:PHE:HE1   | 20       | 1.47          |
| (1,1739) | 1:A:7:LEU:HD23 | 1:A:15:PHE:HE1   | 20       | 1.47          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG21 | 7        | 1.47          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG22 | 7        | 1.47          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG23 | 7        | 1.47          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG21 | 12       | 1.47          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG22 | 12       | 1.47          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG23 | 12       | 1.47          |
| (1,2261) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HD2   | 3        | 1.46          |
| (1,2261) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HD3   | 3        | 1.46          |
| (1,2259) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HG2   | 16       | 1.46          |
| (1,2259) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HG3   | 16       | 1.46          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,2259) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HG2   | 20       | 1.46          |
| (1,2259) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HG3   | 20       | 1.46          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB2   | 6        | 1.46          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB3   | 6        | 1.46          |
| (1,1965) | 1:A:15:PHE:HD2 | 1:A:35:GLY:HA2   | 11       | 1.46          |
| (1,1965) | 1:A:15:PHE:HD2 | 1:A:35:GLY:HA3   | 11       | 1.46          |
| (1,1843) | 1:A:81:SER:HB2 | 1:A:84:TYR:HE1   | 13       | 1.46          |
| (1,1796) | 1:A:31:GLU:H   | 1:A:33:TYR:HE2   | 12       | 1.46          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG21 | 3        | 1.46          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG22 | 3        | 1.46          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG23 | 3        | 1.46          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG21 | 19       | 1.46          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG22 | 19       | 1.46          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG23 | 19       | 1.46          |
| (1,1385) | 1:A:66:PRO:HB2 | 1:A:84:TYR:HD1   | 9        | 1.46          |
| (1,928)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:HA    | 12       | 1.45          |
| (1,928)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:HA    | 14       | 1.45          |
| (1,1965) | 1:A:15:PHE:HD2 | 1:A:35:GLY:HA2   | 4        | 1.45          |
| (1,1965) | 1:A:15:PHE:HD2 | 1:A:35:GLY:HA3   | 4        | 1.45          |
| (1,1841) | 1:A:67:TYR:HA  | 1:A:84:TYR:HE1   | 6        | 1.45          |
| (1,1829) | 1:A:68:PHE:HD2 | 1:A:81:SER:HB3   | 19       | 1.45          |
| (1,928)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:HA    | 15       | 1.44          |
| (1,928)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:HA    | 19       | 1.44          |
| (1,852)  | 1:A:7:LEU:HD21 | 1:A:15:PHE:HD1   | 19       | 1.44          |
| (1,852)  | 1:A:7:LEU:HD22 | 1:A:15:PHE:HD1   | 19       | 1.44          |
| (1,852)  | 1:A:7:LEU:HD23 | 1:A:15:PHE:HD1   | 19       | 1.44          |
| (1,470)  | 1:A:68:PHE:HE2 | 1:A:94:ILE:H     | 16       | 1.44          |
| (1,26)   | 1:A:6:GLU:H    | 1:A:17:PHE:HD1   | 18       | 1.44          |
| (1,2260) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HG2   | 18       | 1.44          |
| (1,2260) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HG3   | 18       | 1.44          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB1   | 6        | 1.44          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB2   | 6        | 1.44          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB3   | 6        | 1.44          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG21 | 10       | 1.44          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG22 | 10       | 1.44          |
| (1,1720) | 1:A:15:PHE:HD1 | 1:A:110:THR:HG23 | 10       | 1.44          |
| (1,1422) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HD11  | 17       | 1.44          |
| (1,1422) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HD12  | 17       | 1.44          |
| (1,1422) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HD13  | 17       | 1.44          |
| (1,1407) | 1:A:67:TYR:HB3 | 1:A:84:TYR:HD1   | 13       | 1.44          |
| (1,26)   | 1:A:6:GLU:H    | 1:A:17:PHE:HD1   | 15       | 1.43          |
| (1,1844) | 1:A:81:SER:HB3 | 1:A:84:TYR:HE1   | 18       | 1.43          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H     | 16       | 1.43          |
| (1,1739) | 1:A:7:LEU:HD21  | 1:A:15:PHE:HE1   | 11       | 1.43          |
| (1,1739) | 1:A:7:LEU:HD22  | 1:A:15:PHE:HE1   | 11       | 1.43          |
| (1,1739) | 1:A:7:LEU:HD23  | 1:A:15:PHE:HE1   | 11       | 1.43          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG21 | 2        | 1.43          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG22 | 2        | 1.43          |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG23 | 2        | 1.43          |
| (1,1407) | 1:A:67:TYR:HB3  | 1:A:84:TYR:HD1   | 14       | 1.43          |
| (1,1407) | 1:A:67:TYR:HB3  | 1:A:84:TYR:HD1   | 20       | 1.43          |
| (1,879)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1   | 3        | 1.42          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2   | 1        | 1.42          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3   | 1        | 1.42          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2   | 4        | 1.42          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3   | 4        | 1.42          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2   | 17       | 1.42          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3   | 17       | 1.42          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA2   | 20       | 1.42          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA3   | 20       | 1.42          |
| (1,1843) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1   | 1        | 1.42          |
| (1,1843) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1   | 8        | 1.42          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2   | 6        | 1.42          |
| (1,1782) | 1:A:16:LYS:HB3  | 1:A:33:TYR:HD2   | 18       | 1.42          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB2   | 8        | 1.41          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB3   | 8        | 1.41          |
| (1,1909) | 1:A:9:LYS:HB2   | 1:A:15:PHE:HE1   | 7        | 1.41          |
| (1,1909) | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1   | 7        | 1.41          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2   | 6        | 1.41          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2   | 6        | 1.41          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2   | 6        | 1.41          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2   | 18       | 1.41          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 4        | 1.41          |
| (1,1802) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 7        | 1.41          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1   | 18       | 1.41          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD11  | 19       | 1.41          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD12  | 19       | 1.41          |
| (1,1422) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HD13  | 19       | 1.41          |
| (1,282)  | 1:A:15:PHE:HD2  | 1:A:36:LYS:H     | 12       | 1.4           |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2   | 13       | 1.4           |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3   | 13       | 1.4           |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2   | 13       | 1.4           |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3   | 13       | 1.4           |
| (1,1814) | 1:A:60:VAL:HA   | 1:A:67:TYR:HE2   | 8        | 1.4           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2   | 4        | 1.4           |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H     | 18       | 1.4           |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG21 | 15       | 1.4           |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG22 | 15       | 1.4           |
| (1,1720) | 1:A:15:PHE:HD1  | 1:A:110:THR:HG23 | 15       | 1.4           |
| (1,26)   | 1:A:6:GLU:H     | 1:A:17:PHE:HD1   | 8        | 1.39          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2   | 7        | 1.39          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3   | 7        | 1.39          |
| (1,2030) | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 17       | 1.39          |
| (1,2030) | 1:A:30:SER:HB3  | 1:A:33:TYR:HE2   | 17       | 1.39          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2   | 12       | 1.38          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3   | 12       | 1.38          |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1   | 12       | 1.38          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG21 | 5        | 1.38          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG22 | 5        | 1.38          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG23 | 5        | 1.38          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 2        | 1.37          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 2        | 1.37          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 2        | 1.37          |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H     | 10       | 1.37          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1   | 7        | 1.37          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2   | 7        | 1.37          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3   | 7        | 1.37          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 16       | 1.36          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 16       | 1.36          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 16       | 1.36          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB2   | 3        | 1.36          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB3   | 3        | 1.36          |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1   | 11       | 1.36          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1   | 20       | 1.36          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2   | 2        | 1.36          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H     | 3        | 1.36          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1   | 9        | 1.36          |
| (1,2245) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1   | 18       | 1.35          |
| (1,2245) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1   | 18       | 1.35          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1   | 4        | 1.35          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB2   | 9        | 1.34          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB3   | 9        | 1.34          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2   | 1        | 1.34          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2   | 1        | 1.34          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1   | 6        | 1.34          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2   | 6        | 1.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3  | 6        | 1.34          |
| (1,1845) | 1:A:82:GLN:H    | 1:A:84:TYR:HE1  | 8        | 1.34          |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1  | 13       | 1.34          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB1  | 1        | 1.34          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB2  | 1        | 1.34          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB3  | 1        | 1.34          |
| (1,879)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1  | 6        | 1.33          |
| (1,852)  | 1:A:7:LEU:HD21  | 1:A:15:PHE:HD1  | 4        | 1.33          |
| (1,852)  | 1:A:7:LEU:HD22  | 1:A:15:PHE:HD1  | 4        | 1.33          |
| (1,852)  | 1:A:7:LEU:HD23  | 1:A:15:PHE:HD1  | 4        | 1.33          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2  | 1        | 1.33          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3  | 1        | 1.33          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2  | 1        | 1.33          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3  | 1        | 1.33          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2  | 11       | 1.33          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 12       | 1.33          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 12       | 1.33          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 12       | 1.33          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2  | 11       | 1.32          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3  | 11       | 1.32          |
| (1,1884) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HB2  | 11       | 1.32          |
| (1,1884) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HB3  | 11       | 1.32          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1  | 18       | 1.32          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2  | 18       | 1.32          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3  | 18       | 1.32          |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1  | 12       | 1.32          |
| (1,1843) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1  | 18       | 1.32          |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H    | 6        | 1.32          |
| (1,852)  | 1:A:7:LEU:HD21  | 1:A:15:PHE:HD1  | 6        | 1.31          |
| (1,852)  | 1:A:7:LEU:HD22  | 1:A:15:PHE:HD1  | 6        | 1.31          |
| (1,852)  | 1:A:7:LEU:HD23  | 1:A:15:PHE:HD1  | 6        | 1.31          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2  | 4        | 1.31          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2  | 4        | 1.31          |
| (1,1822) | 1:A:68:PHE:HE2  | 1:A:81:SER:HB2  | 19       | 1.31          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 10       | 1.31          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2  | 10       | 1.31          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2  | 10       | 1.31          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2  | 17       | 1.31          |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H    | 19       | 1.31          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1  | 4        | 1.31          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1  | 7        | 1.31          |
| (1,26)   | 1:A:6:GLU:H     | 1:A:17:PHE:HD1  | 16       | 1.3           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2260) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HG2  | 12       | 1.3           |
| (1,2260) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HG3  | 12       | 1.3           |
| (1,2260) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HG2  | 16       | 1.3           |
| (1,2260) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HG3  | 16       | 1.3           |
| (1,2259) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HG2  | 9        | 1.3           |
| (1,2259) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HG3  | 9        | 1.3           |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD2  | 6        | 1.3           |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD3  | 6        | 1.3           |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB2  | 11       | 1.3           |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB3  | 11       | 1.3           |
| (1,1963) | 1:A:15:PHE:HE2 | 1:A:35:GLY:HA2  | 19       | 1.3           |
| (1,1963) | 1:A:15:PHE:HE2 | 1:A:35:GLY:HA3  | 19       | 1.3           |
| (1,1909) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HE1  | 10       | 1.3           |
| (1,1909) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 10       | 1.3           |
| (1,1909) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HE1  | 12       | 1.3           |
| (1,1909) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 12       | 1.3           |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB1  | 18       | 1.3           |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB2  | 18       | 1.3           |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB3  | 18       | 1.3           |
| (1,1798) | 1:A:33:TYR:HE1 | 1:A:42:GLY:H    | 10       | 1.3           |
| (1,1798) | 1:A:33:TYR:HE1 | 1:A:42:GLY:H    | 11       | 1.3           |
| (1,1798) | 1:A:33:TYR:HE1 | 1:A:42:GLY:H    | 13       | 1.3           |
| (1,879)  | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 5        | 1.29          |
| (1,26)   | 1:A:6:GLU:H    | 1:A:17:PHE:HD1  | 12       | 1.29          |
| (1,1847) | 1:A:84:TYR:HE2 | 1:A:89:ALA:HB1  | 13       | 1.29          |
| (1,1847) | 1:A:84:TYR:HE2 | 1:A:89:ALA:HB2  | 13       | 1.29          |
| (1,1847) | 1:A:84:TYR:HE2 | 1:A:89:ALA:HB3  | 13       | 1.29          |
| (1,1820) | 1:A:67:TYR:HE1 | 1:A:80:THR:HG21 | 2        | 1.29          |
| (1,1820) | 1:A:67:TYR:HE1 | 1:A:80:THR:HG22 | 2        | 1.29          |
| (1,1820) | 1:A:67:TYR:HE1 | 1:A:80:THR:HG23 | 2        | 1.29          |
| (1,1798) | 1:A:33:TYR:HE1 | 1:A:42:GLY:H    | 5        | 1.29          |
| (1,1798) | 1:A:33:TYR:HE1 | 1:A:42:GLY:H    | 19       | 1.29          |
| (1,1385) | 1:A:66:PRO:HB2 | 1:A:84:TYR:HD1  | 18       | 1.29          |
| (1,838)  | 1:A:7:LEU:HD11 | 1:A:15:PHE:HD1  | 11       | 1.28          |
| (1,838)  | 1:A:7:LEU:HD12 | 1:A:15:PHE:HD1  | 11       | 1.28          |
| (1,838)  | 1:A:7:LEU:HD13 | 1:A:15:PHE:HD1  | 11       | 1.28          |
| (1,838)  | 1:A:7:LEU:HD11 | 1:A:15:PHE:HD1  | 20       | 1.28          |
| (1,838)  | 1:A:7:LEU:HD12 | 1:A:15:PHE:HD1  | 20       | 1.28          |
| (1,838)  | 1:A:7:LEU:HD13 | 1:A:15:PHE:HD1  | 20       | 1.28          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB2  | 13       | 1.28          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB3  | 13       | 1.28          |
| (1,1965) | 1:A:15:PHE:HD2 | 1:A:35:GLY:HA2  | 15       | 1.28          |

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| Key      | Atom-1         | Atom-2           | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1965) | 1:A:15:PHE:HD2 | 1:A:35:GLY:HA3   | 15       | 1.28          |
| (1,1813) | 1:A:60:VAL:H   | 1:A:67:TYR:HE2   | 1        | 1.28          |
| (1,596)  | 1:A:84:TYR:HD2 | 1:A:85:SER:H     | 9        | 1.27          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB1   | 13       | 1.27          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB2   | 13       | 1.27          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB3   | 13       | 1.27          |
| (1,783)  | 1:A:30:SER:HB2 | 1:A:33:TYR:HE2   | 5        | 1.26          |
| (1,26)   | 1:A:6:GLU:H    | 1:A:17:PHE:HD1   | 19       | 1.26          |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD2   | 4        | 1.26          |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD3   | 4        | 1.26          |
| (1,2136) | 1:A:56:TYR:HB2 | 1:A:68:PHE:HD1   | 15       | 1.26          |
| (1,2136) | 1:A:56:TYR:HB3 | 1:A:68:PHE:HD1   | 15       | 1.26          |
| (1,2031) | 1:A:30:SER:HB2 | 1:A:33:TYR:HD2   | 10       | 1.26          |
| (1,2031) | 1:A:30:SER:HB3 | 1:A:33:TYR:HD2   | 10       | 1.26          |
| (1,1963) | 1:A:15:PHE:HE2 | 1:A:35:GLY:HA2   | 3        | 1.26          |
| (1,1963) | 1:A:15:PHE:HE2 | 1:A:35:GLY:HA3   | 3        | 1.26          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB1   | 3        | 1.26          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB2   | 3        | 1.26          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB3   | 3        | 1.26          |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD2   | 20       | 1.25          |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD3   | 20       | 1.25          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB2   | 2        | 1.25          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB3   | 2        | 1.25          |
| (1,1784) | 1:A:33:TYR:H   | 1:A:33:TYR:HD2   | 1        | 1.25          |
| (1,1770) | 1:A:5:TYR:HD2  | 1:A:17:PHE:HD1   | 6        | 1.25          |
| (1,1743) | 1:A:33:TYR:HD1 | 1:A:35:GLY:H     | 11       | 1.25          |
| (1,1634) | 1:A:5:TYR:HD1  | 1:A:103:THR:HG21 | 17       | 1.25          |
| (1,1634) | 1:A:5:TYR:HD1  | 1:A:103:THR:HG22 | 17       | 1.25          |
| (1,1634) | 1:A:5:TYR:HD1  | 1:A:103:THR:HG23 | 17       | 1.25          |
| (1,838)  | 1:A:7:LEU:HD11 | 1:A:15:PHE:HD1   | 15       | 1.24          |
| (1,838)  | 1:A:7:LEU:HD12 | 1:A:15:PHE:HD1   | 15       | 1.24          |
| (1,838)  | 1:A:7:LEU:HD13 | 1:A:15:PHE:HD1   | 15       | 1.24          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB2   | 14       | 1.24          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB3   | 14       | 1.24          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB2   | 15       | 1.24          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB3   | 15       | 1.24          |
| (1,2031) | 1:A:30:SER:HB2 | 1:A:33:TYR:HD2   | 7        | 1.24          |
| (1,2031) | 1:A:30:SER:HB3 | 1:A:33:TYR:HD2   | 7        | 1.24          |
| (1,887)  | 1:A:9:LYS:HG2  | 1:A:15:PHE:HE1   | 12       | 1.23          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB2   | 1        | 1.23          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB3   | 1        | 1.23          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB2   | 5        | 1.23          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB3   | 5        | 1.23          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2   | 8        | 1.23          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2   | 8        | 1.23          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H     | 17       | 1.23          |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1   | 1        | 1.23          |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1   | 15       | 1.23          |
| (1,26)   | 1:A:6:GLU:H     | 1:A:17:PHE:HD1   | 2        | 1.22          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB2   | 10       | 1.22          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB3   | 10       | 1.22          |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1   | 4        | 1.22          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2   | 7        | 1.22          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2   | 7        | 1.22          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2   | 7        | 1.22          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG21 | 11       | 1.22          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG22 | 11       | 1.22          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG23 | 11       | 1.22          |
| (1,879)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1   | 4        | 1.21          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1   | 3        | 1.21          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2   | 3        | 1.21          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3   | 3        | 1.21          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21  | 9        | 1.21          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22  | 9        | 1.21          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23  | 9        | 1.21          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2   | 11       | 1.21          |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1   | 7        | 1.21          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1   | 6        | 1.21          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 14       | 1.2           |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 14       | 1.2           |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 14       | 1.2           |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1   | 11       | 1.2           |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2   | 11       | 1.2           |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3   | 11       | 1.2           |
| (1,1841) | 1:A:67:TYR:HA   | 1:A:84:TYR:HE1   | 7        | 1.2           |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA    | 9        | 1.2           |
| (1,1407) | 1:A:67:TYR:HB3  | 1:A:84:TYR:HD1   | 7        | 1.2           |
| (1,1407) | 1:A:67:TYR:HB3  | 1:A:84:TYR:HD1   | 12       | 1.2           |
| (1,877)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1   | 20       | 1.19          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 10       | 1.19          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2   | 9        | 1.19          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2   | 9        | 1.19          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2   | 9        | 1.19          |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H     | 12       | 1.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H    | 20       | 1.19          |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1  | 2        | 1.19          |
| (1,1770) | 1:A:5:TYR:HD2   | 1:A:17:PHE:HD1  | 18       | 1.19          |
| (1,1385) | 1:A:66:PRO:HB2  | 1:A:84:TYR:HD1  | 7        | 1.19          |
| (1,26)   | 1:A:6:GLU:H     | 1:A:17:PHE:HD1  | 6        | 1.18          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2  | 12       | 1.18          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3  | 12       | 1.18          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB2  | 20       | 1.18          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB3  | 20       | 1.18          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB1  | 4        | 1.18          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB2  | 4        | 1.18          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB3  | 4        | 1.18          |
| (1,1796) | 1:A:31:GLU:H    | 1:A:33:TYR:HE2  | 18       | 1.18          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2  | 2        | 1.18          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 16       | 1.18          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 16       | 1.18          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 16       | 1.18          |
| (1,26)   | 1:A:6:GLU:H     | 1:A:17:PHE:HD1  | 7        | 1.17          |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1  | 9        | 1.17          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 5        | 1.17          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2  | 5        | 1.17          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2  | 5        | 1.17          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2  | 14       | 1.17          |
| (1,877)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1  | 6        | 1.16          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2  | 5        | 1.16          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2  | 5        | 1.16          |
| (1,2031) | 1:A:30:SER:HB2  | 1:A:33:TYR:HD2  | 17       | 1.16          |
| (1,2031) | 1:A:30:SER:HB3  | 1:A:33:TYR:HD2  | 17       | 1.16          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB1  | 7        | 1.16          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB2  | 7        | 1.16          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB3  | 7        | 1.16          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H    | 5        | 1.16          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H    | 9        | 1.16          |
| (1,1180) | 1:A:5:TYR:HD2   | 1:A:43:ILE:HG13 | 16       | 1.16          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2  | 1        | 1.15          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2  | 1        | 1.15          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2  | 1        | 1.15          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA2  | 19       | 1.15          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA3  | 19       | 1.15          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 13       | 1.15          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2  | 13       | 1.15          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2  | 13       | 1.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 17       | 1.15          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2  | 17       | 1.15          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2  | 17       | 1.15          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H    | 3        | 1.15          |
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H    | 8        | 1.15          |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H    | 16       | 1.14          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2  | 7        | 1.14          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3  | 7        | 1.14          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA2  | 3        | 1.14          |
| (1,1965) | 1:A:15:PHE:HD2  | 1:A:35:GLY:HA3  | 3        | 1.14          |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H    | 4        | 1.14          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2  | 8        | 1.13          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2  | 19       | 1.13          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3  | 19       | 1.13          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2  | 18       | 1.13          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3  | 18       | 1.13          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 4        | 1.13          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 4        | 1.13          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 4        | 1.13          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1  | 10       | 1.13          |
| (1,114)  | 1:A:15:PHE:HD1  | 1:A:16:LYS:H    | 6        | 1.13          |
| (1,114)  | 1:A:15:PHE:HD1  | 1:A:16:LYS:H    | 12       | 1.12          |
| (1,879)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1  | 11       | 1.11          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2  | 8        | 1.11          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3  | 8        | 1.11          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB2  | 7        | 1.11          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB3  | 7        | 1.11          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB2  | 18       | 1.11          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB3  | 18       | 1.11          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H    | 18       | 1.11          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H    | 1        | 1.11          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2  | 16       | 1.11          |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H    | 12       | 1.11          |
| (1,1180) | 1:A:5:TYR:HD2   | 1:A:43:ILE:HG13 | 11       | 1.11          |
| (1,114)  | 1:A:15:PHE:HD1  | 1:A:16:LYS:H    | 7        | 1.11          |
| (1,114)  | 1:A:15:PHE:HD1  | 1:A:16:LYS:H    | 10       | 1.11          |
| (1,282)  | 1:A:15:PHE:HD2  | 1:A:36:LYS:H    | 5        | 1.1           |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 3        | 1.1           |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2  | 3        | 1.1           |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2  | 3        | 1.1           |
| (1,1801) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA2  | 4        | 1.1           |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2  | 8        | 1.1           |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1784) | 1:A:33:TYR:H   | 1:A:33:TYR:HD2  | 20       | 1.1           |
| (1,1739) | 1:A:7:LEU:HD21 | 1:A:15:PHE:HE1  | 19       | 1.1           |
| (1,1739) | 1:A:7:LEU:HD22 | 1:A:15:PHE:HE1  | 19       | 1.1           |
| (1,1739) | 1:A:7:LEU:HD23 | 1:A:15:PHE:HE1  | 19       | 1.1           |
| (1,131)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:H    | 15       | 1.1           |
| (1,117)  | 1:A:15:PHE:HE2 | 1:A:36:LYS:H    | 5        | 1.1           |
| (1,114)  | 1:A:15:PHE:HD1 | 1:A:16:LYS:H    | 2        | 1.1           |
| (1,114)  | 1:A:15:PHE:HD1 | 1:A:16:LYS:H    | 20       | 1.1           |
| (1,2136) | 1:A:56:TYR:HB2 | 1:A:68:PHE:HD1  | 13       | 1.09          |
| (1,2136) | 1:A:56:TYR:HB3 | 1:A:68:PHE:HD1  | 13       | 1.09          |
| (1,1784) | 1:A:33:TYR:H   | 1:A:33:TYR:HD2  | 19       | 1.09          |
| (1,1743) | 1:A:33:TYR:HD1 | 1:A:35:GLY:H    | 1        | 1.09          |
| (1,1743) | 1:A:33:TYR:HD1 | 1:A:35:GLY:H    | 16       | 1.09          |
| (1,1407) | 1:A:67:TYR:HB3 | 1:A:84:TYR:HD1  | 9        | 1.09          |
| (1,131)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:H    | 11       | 1.09          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG21 | 4        | 1.09          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG22 | 4        | 1.09          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG23 | 4        | 1.09          |
| (1,879)  | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 2        | 1.08          |
| (1,852)  | 1:A:7:LEU:HD21 | 1:A:15:PHE:HD1  | 7        | 1.08          |
| (1,852)  | 1:A:7:LEU:HD22 | 1:A:15:PHE:HD1  | 7        | 1.08          |
| (1,852)  | 1:A:7:LEU:HD23 | 1:A:15:PHE:HD1  | 7        | 1.08          |
| (1,1845) | 1:A:82:GLN:H   | 1:A:84:TYR:HE1  | 16       | 1.08          |
| (1,1801) | 1:A:33:TYR:HE1 | 1:A:42:GLY:HA2  | 18       | 1.08          |
| (1,1796) | 1:A:31:GLU:H   | 1:A:33:TYR:HE2  | 14       | 1.08          |
| (1,1793) | 1:A:33:TYR:HD1 | 1:A:39:ALA:H    | 10       | 1.08          |
| (1,1784) | 1:A:33:TYR:H   | 1:A:33:TYR:HD2  | 12       | 1.08          |
| (1,1385) | 1:A:66:PRO:HB2 | 1:A:84:TYR:HD1  | 20       | 1.08          |
| (1,596)  | 1:A:84:TYR:HD2 | 1:A:85:SER:H    | 7        | 1.07          |
| (1,1908) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HD1  | 12       | 1.07          |
| (1,1908) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HD1  | 12       | 1.07          |
| (1,1810) | 1:A:67:TYR:HD1 | 1:A:68:PHE:H    | 2        | 1.07          |
| (1,1796) | 1:A:31:GLU:H   | 1:A:33:TYR:HE2  | 15       | 1.07          |
| (1,1793) | 1:A:33:TYR:HD1 | 1:A:39:ALA:H    | 7        | 1.07          |
| (1,1385) | 1:A:66:PRO:HB2 | 1:A:84:TYR:HD1  | 12       | 1.07          |
| (1,131)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:H    | 1        | 1.07          |
| (1,131)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:H    | 18       | 1.07          |
| (1,131)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:H    | 20       | 1.07          |
| (1,596)  | 1:A:84:TYR:HD2 | 1:A:85:SER:H    | 3        | 1.06          |
| (1,26)   | 1:A:6:GLU:H    | 1:A:17:PHE:HD1  | 1        | 1.06          |
| (1,1385) | 1:A:66:PRO:HB2 | 1:A:84:TYR:HD1  | 6        | 1.06          |
| (1,131)  | 1:A:17:PHE:HD1 | 1:A:18:VAL:H    | 14       | 1.06          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H   | 13       | 1.05          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2 | 3        | 1.05          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3 | 3        | 1.05          |
| (1,2200) | 1:A:68:PHE:HE2  | 1:A:93:GLY:HA2 | 16       | 1.05          |
| (1,2200) | 1:A:68:PHE:HE2  | 1:A:93:GLY:HA3 | 16       | 1.05          |
| (1,1923) | 1:A:9:LYS:HD2   | 1:A:15:PHE:HE1 | 10       | 1.05          |
| (1,1923) | 1:A:9:LYS:HD3   | 1:A:15:PHE:HE1 | 10       | 1.05          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H   | 8        | 1.05          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2 | 5        | 1.05          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2 | 6        | 1.05          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2 | 7        | 1.05          |
| (1,1398) | 1:A:66:PRO:HG2  | 1:A:84:TYR:HD1 | 4        | 1.05          |
| (1,131)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:H   | 16       | 1.05          |
| (1,114)  | 1:A:15:PHE:HD1  | 1:A:16:LYS:H   | 4        | 1.05          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2 | 9        | 1.04          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2 | 13       | 1.04          |
| (1,131)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:H   | 7        | 1.04          |
| (1,131)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:H   | 12       | 1.04          |
| (1,114)  | 1:A:15:PHE:HD1  | 1:A:16:LYS:H   | 15       | 1.04          |
| (1,879)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1 | 15       | 1.03          |
| (1,838)  | 1:A:7:LEU:HD11  | 1:A:15:PHE:HD1 | 19       | 1.03          |
| (1,838)  | 1:A:7:LEU:HD12  | 1:A:15:PHE:HD1 | 19       | 1.03          |
| (1,838)  | 1:A:7:LEU:HD13  | 1:A:15:PHE:HD1 | 19       | 1.03          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2 | 10       | 1.03          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3 | 10       | 1.03          |
| (1,2202) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB2 | 19       | 1.03          |
| (1,2202) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB3 | 19       | 1.03          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2 | 20       | 1.03          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2 | 20       | 1.03          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2 | 20       | 1.03          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H   | 1        | 1.03          |
| (1,1406) | 1:A:67:TYR:HB2  | 1:A:84:TYR:HD1 | 4        | 1.03          |
| (1,131)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:H   | 6        | 1.03          |
| (1,131)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:H   | 19       | 1.03          |
| (1,113)  | 1:A:15:PHE:H    | 1:A:15:PHE:HD2 | 5        | 1.03          |
| (1,113)  | 1:A:15:PHE:H    | 1:A:15:PHE:HD2 | 19       | 1.03          |
| (1,887)  | 1:A:9:LYS:HG2   | 1:A:15:PHE:HE1 | 6        | 1.02          |
| (1,838)  | 1:A:7:LEU:HD11  | 1:A:15:PHE:HD1 | 7        | 1.02          |
| (1,838)  | 1:A:7:LEU:HD12  | 1:A:15:PHE:HD1 | 7        | 1.02          |
| (1,838)  | 1:A:7:LEU:HD13  | 1:A:15:PHE:HD1 | 7        | 1.02          |
| (1,1828) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB2 | 17       | 1.02          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2 | 10       | 1.02          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,131)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:H    | 8        | 1.02          |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H    | 8        | 1.01          |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H    | 11       | 1.01          |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H    | 18       | 1.01          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H    | 11       | 1.01          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H    | 14       | 1.01          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2  | 18       | 1.01          |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H    | 15       | 1.01          |
| (1,131)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:H    | 2        | 1.01          |
| (1,131)  | 1:A:17:PHE:HD1  | 1:A:18:VAL:H    | 4        | 1.01          |
| (1,1180) | 1:A:5:TYR:HD2   | 1:A:43:ILE:HG13 | 17       | 1.01          |
| (1,114)  | 1:A:15:PHE:HD1  | 1:A:16:LYS:H    | 19       | 1.01          |
| (1,113)  | 1:A:15:PHE:H    | 1:A:15:PHE:HD2  | 12       | 1.01          |
| (1,878)  | 1:A:9:LYS:HB2   | 1:A:15:PHE:HE1  | 7        | 1.0           |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2  | 20       | 1.0           |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3  | 20       | 1.0           |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB2  | 4        | 1.0           |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB3  | 4        | 1.0           |
| (1,1844) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1  | 10       | 1.0           |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2  | 15       | 1.0           |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H    | 5        | 1.0           |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H    | 14       | 1.0           |
| (1,1398) | 1:A:66:PRO:HG2  | 1:A:84:TYR:HD1  | 11       | 1.0           |
| (1,113)  | 1:A:15:PHE:H    | 1:A:15:PHE:HD2  | 11       | 1.0           |
| (1,877)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1  | 3        | 0.99          |
| (1,852)  | 1:A:7:LEU:HD21  | 1:A:15:PHE:HD1  | 5        | 0.99          |
| (1,852)  | 1:A:7:LEU:HD22  | 1:A:15:PHE:HD1  | 5        | 0.99          |
| (1,852)  | 1:A:7:LEU:HD23  | 1:A:15:PHE:HD1  | 5        | 0.99          |
| (1,775)  | 1:A:60:VAL:HG21 | 1:A:67:TYR:HD2  | 8        | 0.99          |
| (1,775)  | 1:A:60:VAL:HG22 | 1:A:67:TYR:HD2  | 8        | 0.99          |
| (1,775)  | 1:A:60:VAL:HG23 | 1:A:67:TYR:HD2  | 8        | 0.99          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H    | 17       | 0.99          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H    | 13       | 0.99          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H    | 14       | 0.99          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA   | 12       | 0.99          |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H    | 6        | 0.98          |
| (1,2245) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1  | 15       | 0.98          |
| (1,2245) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1  | 15       | 0.98          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB1  | 11       | 0.98          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB2  | 11       | 0.98          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB3  | 11       | 0.98          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 19       | 0.98          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2 | 19       | 0.98          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2 | 19       | 0.98          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H   | 20       | 0.98          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA  | 14       | 0.98          |
| (1,1407) | 1:A:67:TYR:HB3  | 1:A:84:TYR:HD1 | 6        | 0.98          |
| (1,1398) | 1:A:66:PRO:HG2  | 1:A:84:TYR:HD1 | 16       | 0.98          |
| (1,114)  | 1:A:15:PHE:HD1  | 1:A:16:LYS:H   | 3        | 0.98          |
| (1,113)  | 1:A:15:PHE:H    | 1:A:15:PHE:HD2 | 6        | 0.98          |
| (1,852)  | 1:A:7:LEU:HD21  | 1:A:15:PHE:HD1 | 10       | 0.97          |
| (1,852)  | 1:A:7:LEU:HD22  | 1:A:15:PHE:HD1 | 10       | 0.97          |
| (1,852)  | 1:A:7:LEU:HD23  | 1:A:15:PHE:HD1 | 10       | 0.97          |
| (1,838)  | 1:A:7:LEU:HD11  | 1:A:15:PHE:HD1 | 4        | 0.97          |
| (1,838)  | 1:A:7:LEU:HD12  | 1:A:15:PHE:HD1 | 4        | 0.97          |
| (1,838)  | 1:A:7:LEU:HD13  | 1:A:15:PHE:HD1 | 4        | 0.97          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2 | 14       | 0.97          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3 | 14       | 0.97          |
| (1,1842) | 1:A:68:PHE:HE2  | 1:A:84:TYR:HE1 | 5        | 0.97          |
| (1,1829) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB3 | 7        | 0.97          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H   | 10       | 0.97          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H   | 16       | 0.97          |
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H   | 7        | 0.97          |
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H   | 15       | 0.97          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H   | 2        | 0.97          |
| (1,114)  | 1:A:15:PHE:HD1  | 1:A:16:LYS:H   | 11       | 0.97          |
| (1,852)  | 1:A:7:LEU:HD21  | 1:A:15:PHE:HD1 | 2        | 0.96          |
| (1,852)  | 1:A:7:LEU:HD22  | 1:A:15:PHE:HD1 | 2        | 0.96          |
| (1,852)  | 1:A:7:LEU:HD23  | 1:A:15:PHE:HD1 | 2        | 0.96          |
| (1,852)  | 1:A:7:LEU:HD21  | 1:A:15:PHE:HD1 | 12       | 0.96          |
| (1,852)  | 1:A:7:LEU:HD22  | 1:A:15:PHE:HD1 | 12       | 0.96          |
| (1,852)  | 1:A:7:LEU:HD23  | 1:A:15:PHE:HD1 | 12       | 0.96          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB2 | 12       | 0.96          |
| (1,2195) | 1:A:68:PHE:HD1  | 1:A:70:LEU:HB3 | 12       | 0.96          |
| (1,1908) | 1:A:9:LYS:HB2   | 1:A:15:PHE:HD1 | 7        | 0.96          |
| (1,1908) | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1 | 7        | 0.96          |
| (1,1908) | 1:A:9:LYS:HB2   | 1:A:15:PHE:HD1 | 10       | 0.96          |
| (1,1908) | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1 | 10       | 0.96          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H   | 8        | 0.96          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H   | 18       | 0.96          |
| (1,1784) | 1:A:33:TYR:H    | 1:A:33:TYR:HD2 | 14       | 0.96          |
| (1,117)  | 1:A:15:PHE:HE2  | 1:A:36:LYS:H   | 2        | 0.96          |
| (1,114)  | 1:A:15:PHE:HD1  | 1:A:16:LYS:H   | 5        | 0.96          |
| (1,877)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1 | 5        | 0.95          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,838)  | 1:A:7:LEU:HD11  | 1:A:15:PHE:HD1 | 3        | 0.95          |
| (1,838)  | 1:A:7:LEU:HD12  | 1:A:15:PHE:HD1 | 3        | 0.95          |
| (1,838)  | 1:A:7:LEU:HD13  | 1:A:15:PHE:HD1 | 3        | 0.95          |
| (1,37)   | 1:A:5:TYR:HD2   | 1:A:6:GLU:H    | 11       | 0.95          |
| (1,37)   | 1:A:5:TYR:HD2   | 1:A:6:GLU:H    | 16       | 0.95          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2 | 14       | 0.95          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3 | 14       | 0.95          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2 | 5        | 0.95          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3 | 5        | 0.95          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1 | 10       | 0.95          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2 | 10       | 0.95          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3 | 10       | 0.95          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H   | 19       | 0.95          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H   | 19       | 0.95          |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H   | 2        | 0.95          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA  | 1        | 0.95          |
| (1,1398) | 1:A:66:PRO:HG2  | 1:A:84:TYR:HD1 | 9        | 0.95          |
| (1,113)  | 1:A:15:PHE:H    | 1:A:15:PHE:HD2 | 20       | 0.95          |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H   | 11       | 0.94          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H   | 9        | 0.94          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H   | 12       | 0.94          |
| (1,1409) | 1:A:67:TYR:HD1  | 1:A:68:PHE:HA  | 1        | 0.94          |
| (1,113)  | 1:A:15:PHE:H    | 1:A:15:PHE:HD2 | 15       | 0.94          |
| (1,852)  | 1:A:7:LEU:HD21  | 1:A:15:PHE:HD1 | 3        | 0.93          |
| (1,852)  | 1:A:7:LEU:HD22  | 1:A:15:PHE:HD1 | 3        | 0.93          |
| (1,852)  | 1:A:7:LEU:HD23  | 1:A:15:PHE:HD1 | 3        | 0.93          |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H   | 1        | 0.93          |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H   | 4        | 0.93          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2 | 18       | 0.93          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3 | 18       | 0.93          |
| (1,1801) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA2 | 3        | 0.93          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H   | 16       | 0.93          |
| (1,113)  | 1:A:15:PHE:H    | 1:A:15:PHE:HD2 | 4        | 0.93          |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H   | 18       | 0.92          |
| (1,37)   | 1:A:5:TYR:HD2   | 1:A:6:GLU:H    | 17       | 0.92          |
| (1,2136) | 1:A:56:TYR:HB2  | 1:A:68:PHE:HD1 | 8        | 0.92          |
| (1,2136) | 1:A:56:TYR:HB3  | 1:A:68:PHE:HD1 | 8        | 0.92          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2 | 12       | 0.92          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2 | 12       | 0.92          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2 | 12       | 0.92          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2 | 18       | 0.92          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2 | 18       | 0.92          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2   | 18       | 0.92          |
| (1,1813) | 1:A:60:VAL:H    | 1:A:67:TYR:HE2   | 15       | 0.92          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H     | 15       | 0.92          |
| (1,1801) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA2   | 14       | 0.92          |
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H     | 20       | 0.92          |
| (1,1385) | 1:A:66:PRO:HB2  | 1:A:84:TYR:HD1   | 13       | 0.92          |
| (1,113)  | 1:A:15:PHE:H    | 1:A:15:PHE:HD2   | 3        | 0.92          |
| (1,838)  | 1:A:7:LEU:HD11  | 1:A:15:PHE:HD1   | 2        | 0.91          |
| (1,838)  | 1:A:7:LEU:HD12  | 1:A:15:PHE:HD1   | 2        | 0.91          |
| (1,838)  | 1:A:7:LEU:HD13  | 1:A:15:PHE:HD1   | 2        | 0.91          |
| (1,838)  | 1:A:7:LEU:HD11  | 1:A:15:PHE:HD1   | 6        | 0.91          |
| (1,838)  | 1:A:7:LEU:HD12  | 1:A:15:PHE:HD1   | 6        | 0.91          |
| (1,838)  | 1:A:7:LEU:HD13  | 1:A:15:PHE:HD1   | 6        | 0.91          |
| (1,783)  | 1:A:30:SER:HB2  | 1:A:33:TYR:HE2   | 17       | 0.91          |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H     | 15       | 0.91          |
| (1,37)   | 1:A:5:TYR:HD2   | 1:A:6:GLU:H      | 19       | 0.91          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2   | 9        | 0.91          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3   | 9        | 0.91          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG2   | 20       | 0.91          |
| (1,2260) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HG3   | 20       | 0.91          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H     | 4        | 0.91          |
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H     | 2        | 0.91          |
| (1,1798) | 1:A:33:TYR:HE1  | 1:A:42:GLY:H     | 12       | 0.91          |
| (1,1409) | 1:A:67:TYR:HD1  | 1:A:68:PHE:HA    | 2        | 0.91          |
| (1,117)  | 1:A:15:PHE:HE2  | 1:A:36:LYS:H     | 7        | 0.91          |
| (1,1885) | 1:A:5:TYR:HD2   | 1:A:43:ILE:HG12  | 19       | 0.9           |
| (1,1885) | 1:A:5:TYR:HD2   | 1:A:43:ILE:HG13  | 19       | 0.9           |
| (1,1790) | 1:A:33:TYR:HD1  | 1:A:34:THR:H     | 15       | 0.9           |
| (1,1554) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HA    | 10       | 0.9           |
| (1,1398) | 1:A:66:PRO:HG2  | 1:A:84:TYR:HD1   | 8        | 0.9           |
| (1,113)  | 1:A:15:PHE:H    | 1:A:15:PHE:HD2   | 2        | 0.9           |
| (1,26)   | 1:A:6:GLU:H     | 1:A:17:PHE:HD1   | 14       | 0.89          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2   | 15       | 0.89          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2   | 15       | 0.89          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2   | 15       | 0.89          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H     | 5        | 0.89          |
| (1,1743) | 1:A:33:TYR:HD1  | 1:A:35:GLY:H     | 7        | 0.89          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG21 | 16       | 0.89          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG22 | 16       | 0.89          |
| (1,1634) | 1:A:5:TYR:HD1   | 1:A:103:THR:HG23 | 16       | 0.89          |
| (1,1409) | 1:A:67:TYR:HD1  | 1:A:68:PHE:HA    | 14       | 0.89          |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H     | 20       | 0.88          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1801) | 1:A:33:TYR:HE1 | 1:A:42:GLY:HA2  | 16       | 0.88          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 16       | 0.88          |
| (1,1550) | 1:A:84:TYR:HE2 | 1:A:89:ALA:HA   | 16       | 0.88          |
| (1,1180) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HG13 | 5        | 0.88          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB2  | 16       | 0.87          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB3  | 16       | 0.87          |
| (1,1842) | 1:A:68:PHE:HE2 | 1:A:84:TYR:HE1  | 2        | 0.87          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 5        | 0.87          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 18       | 0.87          |
| (1,1739) | 1:A:7:LEU:HD21 | 1:A:15:PHE:HE1  | 6        | 0.87          |
| (1,1739) | 1:A:7:LEU:HD22 | 1:A:15:PHE:HE1  | 6        | 0.87          |
| (1,1739) | 1:A:7:LEU:HD23 | 1:A:15:PHE:HE1  | 6        | 0.87          |
| (1,838)  | 1:A:7:LEU:HD11 | 1:A:15:PHE:HD1  | 12       | 0.86          |
| (1,838)  | 1:A:7:LEU:HD12 | 1:A:15:PHE:HD1  | 12       | 0.86          |
| (1,838)  | 1:A:7:LEU:HD13 | 1:A:15:PHE:HD1  | 12       | 0.86          |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD2  | 18       | 0.86          |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD3  | 18       | 0.86          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB1  | 8        | 0.86          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB2  | 8        | 0.86          |
| (1,1839) | 1:A:84:TYR:HD2 | 1:A:89:ALA:HB3  | 8        | 0.86          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 10       | 0.86          |
| (1,1407) | 1:A:67:TYR:HB3 | 1:A:84:TYR:HD1  | 4        | 0.86          |
| (1,469)  | 1:A:68:PHE:HD1 | 1:A:69:ASN:H    | 3        | 0.85          |
| (1,469)  | 1:A:68:PHE:HD1 | 1:A:69:ASN:H    | 12       | 0.85          |
| (1,469)  | 1:A:68:PHE:HD1 | 1:A:69:ASN:H    | 13       | 0.85          |
| (1,1828) | 1:A:68:PHE:HD2 | 1:A:81:SER:HB2  | 10       | 0.85          |
| (1,1813) | 1:A:60:VAL:H   | 1:A:67:TYR:HE2  | 8        | 0.85          |
| (1,1807) | 1:A:67:TYR:H   | 1:A:67:TYR:HD2  | 7        | 0.85          |
| (1,1398) | 1:A:66:PRO:HG2 | 1:A:84:TYR:HD1  | 14       | 0.85          |
| (1,1398) | 1:A:66:PRO:HG2 | 1:A:84:TYR:HD1  | 15       | 0.85          |
| (1,113)  | 1:A:15:PHE:H   | 1:A:15:PHE:HD2  | 7        | 0.85          |
| (1,282)  | 1:A:15:PHE:HD2 | 1:A:36:LYS:H    | 10       | 0.84          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 7        | 0.84          |
| (1,1409) | 1:A:67:TYR:HD1 | 1:A:68:PHE:HA   | 10       | 0.84          |
| (1,117)  | 1:A:15:PHE:HE2 | 1:A:36:LYS:H    | 20       | 0.84          |
| (1,113)  | 1:A:15:PHE:H   | 1:A:15:PHE:HD2  | 10       | 0.84          |
| (1,469)  | 1:A:68:PHE:HD1 | 1:A:69:ASN:H    | 1        | 0.83          |
| (1,469)  | 1:A:68:PHE:HD1 | 1:A:69:ASN:H    | 4        | 0.83          |
| (1,1923) | 1:A:9:LYS:HD2  | 1:A:15:PHE:HE1  | 12       | 0.83          |
| (1,1923) | 1:A:9:LYS:HD3  | 1:A:15:PHE:HE1  | 12       | 0.83          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 2        | 0.83          |
| (1,1739) | 1:A:7:LEU:HD21 | 1:A:15:PHE:HE1  | 4        | 0.83          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1739) | 1:A:7:LEU:HD22  | 1:A:15:PHE:HE1  | 4        | 0.83          |
| (1,1739) | 1:A:7:LEU:HD23  | 1:A:15:PHE:HE1  | 4        | 0.83          |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H    | 14       | 0.82          |
| (1,37)   | 1:A:5:TYR:HD2   | 1:A:6:GLU:H     | 5        | 0.82          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2  | 9        | 0.82          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3  | 9        | 0.82          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H    | 6        | 0.82          |
| (1,1810) | 1:A:67:TYR:HD1  | 1:A:68:PHE:H    | 13       | 0.82          |
| (1,1807) | 1:A:67:TYR:H    | 1:A:67:TYR:HD2  | 6        | 0.82          |
| (1,1807) | 1:A:67:TYR:H    | 1:A:67:TYR:HD2  | 13       | 0.82          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA   | 15       | 0.82          |
| (1,117)  | 1:A:15:PHE:HE2  | 1:A:36:LYS:H    | 11       | 0.82          |
| (1,878)  | 1:A:9:LYS:HB2   | 1:A:15:PHE:HE1  | 12       | 0.81          |
| (1,877)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1  | 4        | 0.81          |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H    | 5        | 0.81          |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H    | 15       | 0.81          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2  | 2        | 0.81          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3  | 2        | 0.81          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB1  | 10       | 0.81          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB2  | 10       | 0.81          |
| (1,1839) | 1:A:84:TYR:HD2  | 1:A:89:ALA:HB3  | 10       | 0.81          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG21 | 20       | 0.81          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG22 | 20       | 0.81          |
| (1,1820) | 1:A:67:TYR:HE1  | 1:A:80:THR:HG23 | 20       | 0.81          |
| (1,1801) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA2  | 11       | 0.81          |
| (1,1409) | 1:A:67:TYR:HD1  | 1:A:68:PHE:HA   | 8        | 0.81          |
| (1,838)  | 1:A:7:LEU:HD11  | 1:A:15:PHE:HD1  | 5        | 0.8           |
| (1,838)  | 1:A:7:LEU:HD12  | 1:A:15:PHE:HD1  | 5        | 0.8           |
| (1,838)  | 1:A:7:LEU:HD13  | 1:A:15:PHE:HD1  | 5        | 0.8           |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H    | 20       | 0.8           |
| (1,282)  | 1:A:15:PHE:HD2  | 1:A:36:LYS:H    | 7        | 0.8           |
| (1,1554) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HA   | 8        | 0.8           |
| (1,1409) | 1:A:67:TYR:HD1  | 1:A:68:PHE:HA   | 18       | 0.8           |
| (1,1409) | 1:A:67:TYR:HD1  | 1:A:68:PHE:HA   | 20       | 0.8           |
| (1,117)  | 1:A:15:PHE:HE2  | 1:A:36:LYS:H    | 4        | 0.8           |
| (1,877)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1  | 11       | 0.79          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB1  | 8        | 0.79          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB2  | 8        | 0.79          |
| (1,1847) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HB3  | 8        | 0.79          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 11       | 0.79          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2  | 11       | 0.79          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2  | 11       | 0.79          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 3        | 0.79          |
| (1,1409) | 1:A:67:TYR:HD1 | 1:A:68:PHE:HA   | 9        | 0.79          |
| (1,1409) | 1:A:67:TYR:HD1 | 1:A:68:PHE:HA   | 11       | 0.79          |
| (1,469)  | 1:A:68:PHE:HD1 | 1:A:69:ASN:H    | 16       | 0.78          |
| (1,1798) | 1:A:33:TYR:HE1 | 1:A:42:GLY:H    | 6        | 0.78          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 6        | 0.78          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 12       | 0.78          |
| (1,1409) | 1:A:67:TYR:HD1 | 1:A:68:PHE:HA   | 3        | 0.78          |
| (1,878)  | 1:A:9:LYS:HB2  | 1:A:15:PHE:HE1  | 10       | 0.77          |
| (1,595)  | 1:A:84:TYR:H   | 1:A:84:TYR:HD1  | 20       | 0.77          |
| (1,469)  | 1:A:68:PHE:HD1 | 1:A:69:ASN:H    | 8        | 0.77          |
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 17       | 0.77          |
| (1,1909) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HE1  | 3        | 0.77          |
| (1,1909) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 3        | 0.77          |
| (1,1909) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HE1  | 20       | 0.77          |
| (1,1909) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 20       | 0.77          |
| (1,1801) | 1:A:33:TYR:HE1 | 1:A:42:GLY:HA2  | 1        | 0.77          |
| (1,1793) | 1:A:33:TYR:HD1 | 1:A:39:ALA:H    | 12       | 0.77          |
| (1,1409) | 1:A:67:TYR:HD1 | 1:A:68:PHE:HA   | 16       | 0.77          |
| (1,1385) | 1:A:66:PRO:HB2 | 1:A:84:TYR:HD1  | 3        | 0.77          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG21 | 7        | 0.77          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG22 | 7        | 0.77          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG23 | 7        | 0.77          |
| (1,877)  | 1:A:9:LYS:HB3  | 1:A:15:PHE:HD1  | 2        | 0.76          |
| (1,470)  | 1:A:68:PHE:HE2 | 1:A:94:ILE:H    | 1        | 0.76          |
| (1,36)   | 1:A:5:TYR:H    | 1:A:5:TYR:HD1   | 5        | 0.76          |
| (1,36)   | 1:A:5:TYR:H    | 1:A:5:TYR:HD1   | 17       | 0.76          |
| (1,1810) | 1:A:67:TYR:HD1 | 1:A:68:PHE:H    | 7        | 0.76          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 1        | 0.76          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 14       | 0.76          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 20       | 0.76          |
| (1,1773) | 1:A:9:LYS:HA   | 1:A:15:PHE:HD1  | 7        | 0.76          |
| (1,1743) | 1:A:33:TYR:HD1 | 1:A:35:GLY:H    | 20       | 0.76          |
| (1,1739) | 1:A:7:LEU:HD21 | 1:A:15:PHE:HE1  | 10       | 0.76          |
| (1,1739) | 1:A:7:LEU:HD22 | 1:A:15:PHE:HE1  | 10       | 0.76          |
| (1,1739) | 1:A:7:LEU:HD23 | 1:A:15:PHE:HE1  | 10       | 0.76          |
| (1,36)   | 1:A:5:TYR:H    | 1:A:5:TYR:HD1   | 11       | 0.75          |
| (1,1790) | 1:A:33:TYR:HD1 | 1:A:34:THR:H    | 17       | 0.75          |
| (1,1739) | 1:A:7:LEU:HD21 | 1:A:15:PHE:HE1  | 7        | 0.75          |
| (1,1739) | 1:A:7:LEU:HD22 | 1:A:15:PHE:HE1  | 7        | 0.75          |
| (1,1739) | 1:A:7:LEU:HD23 | 1:A:15:PHE:HE1  | 7        | 0.75          |
| (1,1398) | 1:A:66:PRO:HG2 | 1:A:84:TYR:HD1  | 12       | 0.75          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,838)  | 1:A:7:LEU:HD11  | 1:A:15:PHE:HD1 | 10       | 0.74          |
| (1,838)  | 1:A:7:LEU:HD12  | 1:A:15:PHE:HD1 | 10       | 0.74          |
| (1,838)  | 1:A:7:LEU:HD13  | 1:A:15:PHE:HD1 | 10       | 0.74          |
| (1,468)  | 1:A:68:PHE:H    | 1:A:68:PHE:HD2 | 19       | 0.74          |
| (1,2136) | 1:A:56:TYR:HB2  | 1:A:68:PHE:HD1 | 3        | 0.74          |
| (1,2136) | 1:A:56:TYR:HB3  | 1:A:68:PHE:HD1 | 3        | 0.74          |
| (1,1843) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1 | 7        | 0.74          |
| (1,1739) | 1:A:7:LEU:HD21  | 1:A:15:PHE:HE1 | 2        | 0.74          |
| (1,1739) | 1:A:7:LEU:HD22  | 1:A:15:PHE:HE1 | 2        | 0.74          |
| (1,1739) | 1:A:7:LEU:HD23  | 1:A:15:PHE:HE1 | 2        | 0.74          |
| (1,36)   | 1:A:5:TYR:H     | 1:A:5:TYR:HD1  | 19       | 0.73          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2 | 15       | 0.73          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3 | 15       | 0.73          |
| (1,1840) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HA  | 10       | 0.73          |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1 | 10       | 0.73          |
| (1,1409) | 1:A:67:TYR:HD1  | 1:A:68:PHE:HA  | 12       | 0.73          |
| (1,117)  | 1:A:15:PHE:HE2  | 1:A:36:LYS:H   | 6        | 0.73          |
| (1,887)  | 1:A:9:LYS:HG2   | 1:A:15:PHE:HE1 | 7        | 0.72          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2 | 16       | 0.72          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3 | 16       | 0.72          |
| (1,2199) | 1:A:68:PHE:HE2  | 1:A:81:SER:HB2 | 7        | 0.72          |
| (1,2199) | 1:A:68:PHE:HE2  | 1:A:81:SER:HB3 | 7        | 0.72          |
| (1,1845) | 1:A:82:GLN:H    | 1:A:84:TYR:HE1 | 20       | 0.72          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2 | 16       | 0.72          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2 | 16       | 0.72          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2 | 16       | 0.72          |
| (1,1790) | 1:A:33:TYR:HD1  | 1:A:34:THR:H   | 9        | 0.72          |
| (1,1790) | 1:A:33:TYR:HD1  | 1:A:34:THR:H   | 19       | 0.72          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA  | 4        | 0.72          |
| (1,1407) | 1:A:67:TYR:HB3  | 1:A:84:TYR:HD1 | 10       | 0.72          |
| (1,596)  | 1:A:84:TYR:HD2  | 1:A:85:SER:H   | 14       | 0.71          |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H   | 10       | 0.71          |
| (1,468)  | 1:A:68:PHE:H    | 1:A:68:PHE:HD2 | 3        | 0.71          |
| (1,468)  | 1:A:68:PHE:H    | 1:A:68:PHE:HD2 | 7        | 0.71          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2 | 16       | 0.71          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3 | 16       | 0.71          |
| (1,117)  | 1:A:15:PHE:HE2  | 1:A:36:LYS:H   | 10       | 0.71          |
| (1,877)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1 | 15       | 0.7           |
| (1,468)  | 1:A:68:PHE:H    | 1:A:68:PHE:HD2 | 16       | 0.7           |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2 | 9        | 0.7           |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2 | 9        | 0.7           |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2 | 9        | 0.7           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1793) | 1:A:33:TYR:HD1  | 1:A:39:ALA:H    | 11       | 0.7           |
| (1,1790) | 1:A:33:TYR:HD1  | 1:A:34:THR:H    | 11       | 0.7           |
| (1,1523) | 1:A:81:SER:HA   | 1:A:84:TYR:HE1  | 7        | 0.7           |
| (1,1409) | 1:A:67:TYR:HD1  | 1:A:68:PHE:HA   | 4        | 0.7           |
| (1,1398) | 1:A:66:PRO:HG2  | 1:A:84:TYR:HD1  | 7        | 0.7           |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H    | 17       | 0.69          |
| (1,1917) | 1:A:9:LYS:HG2   | 1:A:15:PHE:HE1  | 10       | 0.69          |
| (1,1917) | 1:A:9:LYS:HG3   | 1:A:15:PHE:HE1  | 10       | 0.69          |
| (1,1807) | 1:A:67:TYR:H    | 1:A:67:TYR:HD2  | 17       | 0.69          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA   | 7        | 0.69          |
| (1,116)  | 1:A:15:PHE:H    | 1:A:15:PHE:HE2  | 12       | 0.69          |
| (1,1739) | 1:A:7:LEU:HD21  | 1:A:15:PHE:HE1  | 12       | 0.68          |
| (1,1739) | 1:A:7:LEU:HD22  | 1:A:15:PHE:HE1  | 12       | 0.68          |
| (1,1739) | 1:A:7:LEU:HD23  | 1:A:15:PHE:HE1  | 12       | 0.68          |
| (1,1385) | 1:A:66:PRO:HB2  | 1:A:84:TYR:HD1  | 1        | 0.68          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 2        | 0.67          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2  | 2        | 0.67          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2  | 2        | 0.67          |
| (1,1807) | 1:A:67:TYR:H    | 1:A:67:TYR:HD2  | 19       | 0.67          |
| (1,1790) | 1:A:33:TYR:HD1  | 1:A:34:THR:H    | 8        | 0.67          |
| (1,1790) | 1:A:33:TYR:HD1  | 1:A:34:THR:H    | 13       | 0.67          |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H    | 7        | 0.66          |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H    | 19       | 0.66          |
| (1,282)  | 1:A:15:PHE:HD2  | 1:A:36:LYS:H    | 2        | 0.66          |
| (1,1801) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA2  | 9        | 0.66          |
| (1,1790) | 1:A:33:TYR:HD1  | 1:A:34:THR:H    | 4        | 0.66          |
| (1,116)  | 1:A:15:PHE:H    | 1:A:15:PHE:HE2  | 19       | 0.66          |
| (1,595)  | 1:A:84:TYR:H    | 1:A:84:TYR:HD1  | 1        | 0.65          |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H    | 2        | 0.65          |
| (1,468)  | 1:A:68:PHE:H    | 1:A:68:PHE:HD2  | 14       | 0.65          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD2  | 14       | 0.65          |
| (1,2261) | 1:A:84:TYR:HE1  | 1:A:90:ARG:HD3  | 14       | 0.65          |
| (1,1828) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB2  | 9        | 0.65          |
| (1,117)  | 1:A:15:PHE:HE2  | 1:A:36:LYS:H    | 15       | 0.65          |
| (1,116)  | 1:A:15:PHE:H    | 1:A:15:PHE:HE2  | 6        | 0.65          |
| (1,595)  | 1:A:84:TYR:H    | 1:A:84:TYR:HD1  | 3        | 0.64          |
| (1,36)   | 1:A:5:TYR:H     | 1:A:5:TYR:HD1   | 16       | 0.64          |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG21 | 14       | 0.64          |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG22 | 14       | 0.64          |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG23 | 14       | 0.64          |
| (1,116)  | 1:A:15:PHE:H    | 1:A:15:PHE:HE2  | 5        | 0.64          |
| (1,116)  | 1:A:15:PHE:H    | 1:A:15:PHE:HE2  | 11       | 0.64          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 12       | 0.63          |
| (1,1828) | 1:A:68:PHE:HD2 | 1:A:81:SER:HB2  | 19       | 0.63          |
| (1,1801) | 1:A:33:TYR:HE1 | 1:A:42:GLY:HA2  | 19       | 0.63          |
| (1,1773) | 1:A:9:LYS:HA   | 1:A:15:PHE:HD1  | 10       | 0.63          |
| (1,595)  | 1:A:84:TYR:H   | 1:A:84:TYR:HD1  | 6        | 0.62          |
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 5        | 0.62          |
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 10       | 0.62          |
| (1,1409) | 1:A:67:TYR:HD1 | 1:A:68:PHE:HA   | 15       | 0.62          |
| (1,117)  | 1:A:15:PHE:HE2 | 1:A:36:LYS:H    | 19       | 0.62          |
| (1,595)  | 1:A:84:TYR:H   | 1:A:84:TYR:HD1  | 15       | 0.61          |
| (1,1828) | 1:A:68:PHE:HD2 | 1:A:81:SER:HB2  | 8        | 0.61          |
| (1,1409) | 1:A:67:TYR:HD1 | 1:A:68:PHE:HA   | 17       | 0.61          |
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 1        | 0.6           |
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 6        | 0.6           |
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 11       | 0.6           |
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 18       | 0.6           |
| (1,282)  | 1:A:15:PHE:HD2 | 1:A:36:LYS:H    | 6        | 0.6           |
| (1,2136) | 1:A:56:TYR:HB2 | 1:A:68:PHE:HD1  | 1        | 0.6           |
| (1,2136) | 1:A:56:TYR:HB3 | 1:A:68:PHE:HD1  | 1        | 0.6           |
| (1,1845) | 1:A:82:GLN:H   | 1:A:84:TYR:HE1  | 3        | 0.6           |
| (1,1823) | 1:A:68:PHE:HE2 | 1:A:81:SER:HB3  | 7        | 0.6           |
| (1,1807) | 1:A:67:TYR:H   | 1:A:67:TYR:HD2  | 5        | 0.6           |
| (1,1803) | 1:A:33:TYR:HE1 | 1:A:39:ALA:HA   | 4        | 0.6           |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG21 | 10       | 0.6           |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG22 | 10       | 0.6           |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG23 | 10       | 0.6           |
| (1,595)  | 1:A:84:TYR:H   | 1:A:84:TYR:HD1  | 11       | 0.59          |
| (1,469)  | 1:A:68:PHE:HD1 | 1:A:69:ASN:H    | 9        | 0.59          |
| (1,1554) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HA   | 15       | 0.59          |
| (1,116)  | 1:A:15:PHE:H   | 1:A:15:PHE:HE2  | 20       | 0.59          |
| (1,1909) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HE1  | 5        | 0.58          |
| (1,1909) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 5        | 0.58          |
| (1,1828) | 1:A:68:PHE:HD2 | 1:A:81:SER:HB2  | 11       | 0.58          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG21 | 3        | 0.58          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG22 | 3        | 0.58          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG23 | 3        | 0.58          |
| (1,1398) | 1:A:66:PRO:HG2 | 1:A:84:TYR:HD1  | 6        | 0.58          |
| (1,595)  | 1:A:84:TYR:H   | 1:A:84:TYR:HD1  | 14       | 0.57          |
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 9        | 0.57          |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG2  | 1        | 0.57          |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG3  | 1        | 0.57          |
| (1,1807) | 1:A:67:TYR:H   | 1:A:67:TYR:HD2  | 15       | 0.57          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1801) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA2  | 13       | 0.57          |
| (1,1801) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA2  | 17       | 0.57          |
| (1,1398) | 1:A:66:PRO:HG2  | 1:A:84:TYR:HD1  | 18       | 0.57          |
| (1,595)  | 1:A:84:TYR:H    | 1:A:84:TYR:HD1  | 4        | 0.56          |
| (1,469)  | 1:A:68:PHE:HD1  | 1:A:69:ASN:H    | 6        | 0.56          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA   | 6        | 0.56          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA   | 13       | 0.56          |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG21 | 6        | 0.56          |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG22 | 6        | 0.56          |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG23 | 6        | 0.56          |
| (1,887)  | 1:A:9:LYS:HG2   | 1:A:15:PHE:HE1  | 20       | 0.55          |
| (1,595)  | 1:A:84:TYR:H    | 1:A:84:TYR:HD1  | 8        | 0.55          |
| (1,595)  | 1:A:84:TYR:H    | 1:A:84:TYR:HD1  | 13       | 0.55          |
| (1,595)  | 1:A:84:TYR:H    | 1:A:84:TYR:HD1  | 16       | 0.55          |
| (1,282)  | 1:A:15:PHE:HD2  | 1:A:36:LYS:H    | 4        | 0.55          |
| (1,1822) | 1:A:68:PHE:HE2  | 1:A:81:SER:HB2  | 17       | 0.55          |
| (1,1739) | 1:A:7:LEU:HD21  | 1:A:15:PHE:HE1  | 5        | 0.55          |
| (1,1739) | 1:A:7:LEU:HD22  | 1:A:15:PHE:HE1  | 5        | 0.55          |
| (1,1739) | 1:A:7:LEU:HD23  | 1:A:15:PHE:HE1  | 5        | 0.55          |
| (1,1409) | 1:A:67:TYR:HD1  | 1:A:68:PHE:HA   | 5        | 0.55          |
| (1,116)  | 1:A:15:PHE:H    | 1:A:15:PHE:HE2  | 4        | 0.55          |
| (1,116)  | 1:A:15:PHE:H    | 1:A:15:PHE:HE2  | 15       | 0.55          |
| (1,468)  | 1:A:68:PHE:H    | 1:A:68:PHE:HD2  | 8        | 0.54          |
| (1,2200) | 1:A:68:PHE:HE2  | 1:A:93:GLY:HA2  | 1        | 0.54          |
| (1,2200) | 1:A:68:PHE:HE2  | 1:A:93:GLY:HA3  | 1        | 0.54          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 1        | 0.54          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2  | 1        | 0.54          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2  | 1        | 0.54          |
| (1,1807) | 1:A:67:TYR:H    | 1:A:67:TYR:HD2  | 8        | 0.54          |
| (1,1739) | 1:A:7:LEU:HD21  | 1:A:15:PHE:HE1  | 3        | 0.54          |
| (1,1739) | 1:A:7:LEU:HD22  | 1:A:15:PHE:HE1  | 3        | 0.54          |
| (1,1739) | 1:A:7:LEU:HD23  | 1:A:15:PHE:HE1  | 3        | 0.54          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA   | 18       | 0.54          |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG21 | 1        | 0.54          |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG22 | 1        | 0.54          |
| (1,1184) | 1:A:17:PHE:HD1  | 1:A:43:ILE:HG23 | 1        | 0.54          |
| (1,468)  | 1:A:68:PHE:H    | 1:A:68:PHE:HD2  | 13       | 0.53          |
| (1,282)  | 1:A:15:PHE:HD2  | 1:A:36:LYS:H    | 11       | 0.53          |
| (1,2245) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1  | 6        | 0.53          |
| (1,2245) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1  | 6        | 0.53          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2  | 8        | 0.53          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3  | 8        | 0.53          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1807) | 1:A:67:TYR:H   | 1:A:67:TYR:HD2  | 4        | 0.53          |
| (1,1799) | 1:A:33:TYR:HE1 | 1:A:42:GLY:HA3  | 4        | 0.53          |
| (1,1588) | 1:A:68:PHE:HD2 | 1:A:94:ILE:HG13 | 17       | 0.53          |
| (1,595)  | 1:A:84:TYR:H   | 1:A:84:TYR:HD1  | 12       | 0.52          |
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 4        | 0.52          |
| (1,116)  | 1:A:15:PHE:H   | 1:A:15:PHE:HE2  | 3        | 0.52          |
| (1,1909) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HE1  | 4        | 0.51          |
| (1,1909) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 4        | 0.51          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 15       | 0.51          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 20       | 0.51          |
| (1,117)  | 1:A:15:PHE:HE2 | 1:A:36:LYS:H    | 3        | 0.51          |
| (1,842)  | 1:A:7:LEU:HD11 | 1:A:17:PHE:HD2  | 15       | 0.5           |
| (1,842)  | 1:A:7:LEU:HD12 | 1:A:17:PHE:HD2  | 15       | 0.5           |
| (1,842)  | 1:A:7:LEU:HD13 | 1:A:17:PHE:HD2  | 15       | 0.5           |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB2  | 19       | 0.5           |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB3  | 19       | 0.5           |
| (1,1398) | 1:A:66:PRO:HG2 | 1:A:84:TYR:HD1  | 20       | 0.5           |
| (1,116)  | 1:A:15:PHE:H   | 1:A:15:PHE:HE2  | 2        | 0.5           |
| (1,282)  | 1:A:15:PHE:HD2 | 1:A:36:LYS:H    | 20       | 0.49          |
| (1,1845) | 1:A:82:GLN:H   | 1:A:84:TYR:HE1  | 1        | 0.49          |
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 10       | 0.49          |
| (1,1807) | 1:A:67:TYR:H   | 1:A:67:TYR:HD2  | 10       | 0.49          |
| (1,1793) | 1:A:33:TYR:HD1 | 1:A:39:ALA:H    | 15       | 0.49          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG21 | 9        | 0.49          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG22 | 9        | 0.49          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG23 | 9        | 0.49          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 1        | 0.49          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 2        | 0.49          |
| (1,1409) | 1:A:67:TYR:HD1 | 1:A:68:PHE:HA   | 19       | 0.49          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB2  | 17       | 0.48          |
| (1,2195) | 1:A:68:PHE:HD1 | 1:A:70:LEU:HB3  | 17       | 0.48          |
| (1,1807) | 1:A:67:TYR:H   | 1:A:67:TYR:HD2  | 12       | 0.48          |
| (1,1801) | 1:A:33:TYR:HE1 | 1:A:42:GLY:HA2  | 15       | 0.48          |
| (1,1793) | 1:A:33:TYR:HD1 | 1:A:39:ALA:H    | 6        | 0.48          |
| (1,1423) | 1:A:68:PHE:HE1 | 1:A:70:LEU:HD11 | 17       | 0.48          |
| (1,1423) | 1:A:68:PHE:HE1 | 1:A:70:LEU:HD12 | 17       | 0.48          |
| (1,1423) | 1:A:68:PHE:HE1 | 1:A:70:LEU:HD13 | 17       | 0.48          |
| (1,887)  | 1:A:9:LYS:HG2  | 1:A:15:PHE:HE1  | 4        | 0.47          |
| (1,876)  | 1:A:9:LYS:HB2  | 1:A:15:PHE:HD1  | 12       | 0.47          |
| (1,595)  | 1:A:84:TYR:H   | 1:A:84:TYR:HD1  | 9        | 0.47          |
| (1,1843) | 1:A:81:SER:HB2 | 1:A:84:TYR:HE1  | 15       | 0.47          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 5        | 0.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1909) | 1:A:9:LYS:HB2   | 1:A:15:PHE:HE1  | 11       | 0.46          |
| (1,1909) | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1  | 11       | 0.46          |
| (1,1828) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB2  | 4        | 0.46          |
| (1,1773) | 1:A:9:LYS:HA    | 1:A:15:PHE:HD1  | 4        | 0.46          |
| (1,116)  | 1:A:15:PHE:H    | 1:A:15:PHE:HE2  | 7        | 0.46          |
| (1,282)  | 1:A:15:PHE:HD2  | 1:A:36:LYS:H    | 19       | 0.45          |
| (1,258)  | 1:A:15:PHE:H    | 1:A:33:TYR:HD2  | 11       | 0.45          |
| (1,2202) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB2  | 7        | 0.45          |
| (1,2202) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB3  | 7        | 0.45          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 14       | 0.45          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2  | 14       | 0.45          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2  | 14       | 0.45          |
| (1,1803) | 1:A:33:TYR:HE1  | 1:A:39:ALA:HA   | 3        | 0.45          |
| (1,1773) | 1:A:9:LYS:HA    | 1:A:15:PHE:HD1  | 20       | 0.45          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA   | 3        | 0.45          |
| (1,1413) | 1:A:68:PHE:HD1  | 1:A:69:ASN:HA   | 4        | 0.45          |
| (1,595)  | 1:A:84:TYR:H    | 1:A:84:TYR:HD1  | 18       | 0.44          |
| (1,1908) | 1:A:9:LYS:HB2   | 1:A:15:PHE:HD1  | 20       | 0.44          |
| (1,1908) | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1  | 20       | 0.44          |
| (1,1773) | 1:A:9:LYS:HA    | 1:A:15:PHE:HD1  | 12       | 0.44          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD11 | 19       | 0.44          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD12 | 19       | 0.44          |
| (1,1423) | 1:A:68:PHE:HE1  | 1:A:70:LEU:HD13 | 19       | 0.44          |
| (1,879)  | 1:A:9:LYS:HB3   | 1:A:15:PHE:HE1  | 19       | 0.43          |
| (1,842)  | 1:A:7:LEU:HD11  | 1:A:17:PHE:HD2  | 20       | 0.43          |
| (1,842)  | 1:A:7:LEU:HD12  | 1:A:17:PHE:HD2  | 20       | 0.43          |
| (1,842)  | 1:A:7:LEU:HD13  | 1:A:17:PHE:HD2  | 20       | 0.43          |
| (1,468)  | 1:A:68:PHE:H    | 1:A:68:PHE:HD2  | 15       | 0.43          |
| (1,1885) | 1:A:5:TYR:HD2   | 1:A:43:ILE:HG12 | 16       | 0.43          |
| (1,1885) | 1:A:5:TYR:HD2   | 1:A:43:ILE:HG13 | 16       | 0.43          |
| (1,1807) | 1:A:67:TYR:H    | 1:A:67:TYR:HD2  | 9        | 0.43          |
| (1,116)  | 1:A:15:PHE:H    | 1:A:15:PHE:HE2  | 10       | 0.43          |
| (1,258)  | 1:A:15:PHE:H    | 1:A:33:TYR:HD2  | 16       | 0.42          |
| (1,258)  | 1:A:15:PHE:H    | 1:A:33:TYR:HD2  | 19       | 0.42          |
| (1,2245) | 1:A:81:SER:HB2  | 1:A:84:TYR:HE1  | 11       | 0.42          |
| (1,2245) | 1:A:81:SER:HB3  | 1:A:84:TYR:HE1  | 11       | 0.42          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG11 | 6        | 0.42          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG12 | 6        | 0.42          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG13 | 6        | 0.42          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG21 | 6        | 0.42          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG22 | 6        | 0.42          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG23 | 6        | 0.42          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 11       | 0.42          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 13       | 0.42          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 18       | 0.42          |
| (1,1409) | 1:A:67:TYR:HD1 | 1:A:68:PHE:HA   | 6        | 0.42          |
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 2        | 0.41          |
| (1,1927) | 1:A:9:LYS:HE2  | 1:A:15:PHE:HE1  | 2        | 0.41          |
| (1,1927) | 1:A:9:LYS:HE3  | 1:A:15:PHE:HE1  | 2        | 0.41          |
| (1,1807) | 1:A:67:TYR:H   | 1:A:67:TYR:HD2  | 18       | 0.41          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG21 | 16       | 0.41          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG22 | 16       | 0.41          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG23 | 16       | 0.41          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG21 | 20       | 0.41          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG22 | 20       | 0.41          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG23 | 20       | 0.41          |
| (1,468)  | 1:A:68:PHE:H   | 1:A:68:PHE:HD2  | 20       | 0.4           |
| (1,1807) | 1:A:67:TYR:H   | 1:A:67:TYR:HD2  | 3        | 0.4           |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 12       | 0.4           |
| (1,842)  | 1:A:7:LEU:HD11 | 1:A:17:PHE:HD2  | 12       | 0.39          |
| (1,842)  | 1:A:7:LEU:HD12 | 1:A:17:PHE:HD2  | 12       | 0.39          |
| (1,842)  | 1:A:7:LEU:HD13 | 1:A:17:PHE:HD2  | 12       | 0.39          |
| (1,842)  | 1:A:7:LEU:HD11 | 1:A:17:PHE:HD2  | 14       | 0.39          |
| (1,842)  | 1:A:7:LEU:HD12 | 1:A:17:PHE:HD2  | 14       | 0.39          |
| (1,842)  | 1:A:7:LEU:HD13 | 1:A:17:PHE:HD2  | 14       | 0.39          |
| (1,595)  | 1:A:84:TYR:H   | 1:A:84:TYR:HD1  | 7        | 0.39          |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD2  | 14       | 0.39          |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD3  | 14       | 0.39          |
| (1,1807) | 1:A:67:TYR:H   | 1:A:67:TYR:HD2  | 16       | 0.39          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG21 | 6        | 0.39          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG22 | 6        | 0.39          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG23 | 6        | 0.39          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG21 | 11       | 0.39          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG22 | 11       | 0.39          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG23 | 11       | 0.39          |
| (1,876)  | 1:A:9:LYS:HB2  | 1:A:15:PHE:HD1  | 7        | 0.38          |
| (1,842)  | 1:A:7:LEU:HD11 | 1:A:17:PHE:HD2  | 6        | 0.38          |
| (1,842)  | 1:A:7:LEU:HD12 | 1:A:17:PHE:HD2  | 6        | 0.38          |
| (1,842)  | 1:A:7:LEU:HD13 | 1:A:17:PHE:HD2  | 6        | 0.38          |
| (1,842)  | 1:A:7:LEU:HD11 | 1:A:17:PHE:HD2  | 11       | 0.38          |
| (1,842)  | 1:A:7:LEU:HD12 | 1:A:17:PHE:HD2  | 11       | 0.38          |
| (1,842)  | 1:A:7:LEU:HD13 | 1:A:17:PHE:HD2  | 11       | 0.38          |
| (1,258)  | 1:A:15:PHE:H   | 1:A:33:TYR:HD2  | 13       | 0.38          |
| (1,1908) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HD1  | 3        | 0.38          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1908) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HD1  | 3        | 0.38          |
| (1,1840) | 1:A:84:TYR:HD1 | 1:A:90:ARG:HA   | 8        | 0.38          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG21 | 2        | 0.38          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG22 | 2        | 0.38          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG23 | 2        | 0.38          |
| (1,258)  | 1:A:15:PHE:H   | 1:A:33:TYR:HD2  | 14       | 0.37          |
| (1,1927) | 1:A:9:LYS:HE2  | 1:A:15:PHE:HE1  | 3        | 0.37          |
| (1,1927) | 1:A:9:LYS:HE3  | 1:A:15:PHE:HE1  | 3        | 0.37          |
| (1,1927) | 1:A:9:LYS:HE2  | 1:A:15:PHE:HE1  | 7        | 0.37          |
| (1,1927) | 1:A:9:LYS:HE3  | 1:A:15:PHE:HE1  | 7        | 0.37          |
| (1,1909) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HE1  | 2        | 0.37          |
| (1,1909) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 2        | 0.37          |
| (1,1909) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HE1  | 15       | 0.37          |
| (1,1909) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 15       | 0.37          |
| (1,1885) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HG12 | 11       | 0.37          |
| (1,1885) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HG13 | 11       | 0.37          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 9        | 0.37          |
| (1,470)  | 1:A:68:PHE:HE2 | 1:A:94:ILE:H    | 18       | 0.36          |
| (1,470)  | 1:A:68:PHE:HE2 | 1:A:94:ILE:H    | 20       | 0.36          |
| (1,258)  | 1:A:15:PHE:H   | 1:A:33:TYR:HD2  | 12       | 0.36          |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG2  | 4        | 0.36          |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG3  | 4        | 0.36          |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG2  | 20       | 0.36          |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG3  | 20       | 0.36          |
| (1,1909) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HE1  | 6        | 0.36          |
| (1,1909) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HE1  | 6        | 0.36          |
| (1,1828) | 1:A:68:PHE:HD2 | 1:A:81:SER:HB2  | 6        | 0.36          |
| (1,1773) | 1:A:9:LYS:HA   | 1:A:15:PHE:HD1  | 3        | 0.36          |
| (1,1588) | 1:A:68:PHE:HD2 | 1:A:94:ILE:HG13 | 19       | 0.36          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 16       | 0.36          |
| (1,1409) | 1:A:67:TYR:HD1 | 1:A:68:PHE:HA   | 13       | 0.36          |
| (1,1169) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HD11 | 19       | 0.36          |
| (1,1169) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HD12 | 19       | 0.36          |
| (1,1169) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HD13 | 19       | 0.36          |
| (1,842)  | 1:A:7:LEU:HD11 | 1:A:17:PHE:HD2  | 8        | 0.35          |
| (1,842)  | 1:A:7:LEU:HD12 | 1:A:17:PHE:HD2  | 8        | 0.35          |
| (1,842)  | 1:A:7:LEU:HD13 | 1:A:17:PHE:HD2  | 8        | 0.35          |
| (1,1807) | 1:A:67:TYR:H   | 1:A:67:TYR:HD2  | 11       | 0.35          |
| (1,258)  | 1:A:15:PHE:H   | 1:A:33:TYR:HD2  | 4        | 0.34          |
| (1,258)  | 1:A:15:PHE:H   | 1:A:33:TYR:HD2  | 15       | 0.34          |
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 7        | 0.34          |
| (1,1801) | 1:A:33:TYR:HE1 | 1:A:42:GLY:HA2  | 10       | 0.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA   | 11       | 0.34          |
| (1,1413) | 1:A:68:PHE:HD1  | 1:A:69:ASN:HA   | 3        | 0.34          |
| (1,1179) | 1:A:5:TYR:HD2   | 1:A:43:ILE:HG12 | 19       | 0.34          |
| (1,842)  | 1:A:7:LEU:HD11  | 1:A:17:PHE:HD2  | 18       | 0.33          |
| (1,842)  | 1:A:7:LEU:HD12  | 1:A:17:PHE:HD2  | 18       | 0.33          |
| (1,842)  | 1:A:7:LEU:HD13  | 1:A:17:PHE:HD2  | 18       | 0.33          |
| (1,282)  | 1:A:15:PHE:HD2  | 1:A:36:LYS:H    | 3        | 0.33          |
| (1,258)  | 1:A:15:PHE:H    | 1:A:33:TYR:HD2  | 6        | 0.33          |
| (1,1819) | 1:A:60:VAL:HG21 | 1:A:67:TYR:HE2  | 8        | 0.33          |
| (1,1819) | 1:A:60:VAL:HG22 | 1:A:67:TYR:HE2  | 8        | 0.33          |
| (1,1819) | 1:A:60:VAL:HG23 | 1:A:67:TYR:HE2  | 8        | 0.33          |
| (1,1801) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA2  | 20       | 0.33          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2  | 13       | 0.32          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3  | 13       | 0.32          |
| (1,1845) | 1:A:82:GLN:H    | 1:A:84:TYR:HE1  | 6        | 0.32          |
| (1,1807) | 1:A:67:TYR:H    | 1:A:67:TYR:HD2  | 1        | 0.32          |
| (1,1807) | 1:A:67:TYR:H    | 1:A:67:TYR:HD2  | 14       | 0.32          |
| (1,1799) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA3  | 3        | 0.32          |
| (1,1771) | 1:A:15:PHE:HD2  | 1:A:36:LYS:HA   | 12       | 0.32          |
| (1,1550) | 1:A:84:TYR:HE2  | 1:A:89:ALA:HA   | 10       | 0.32          |
| (1,1413) | 1:A:68:PHE:HD1  | 1:A:69:ASN:HA   | 8        | 0.32          |
| (1,876)  | 1:A:9:LYS:HB2   | 1:A:15:PHE:HD1  | 10       | 0.31          |
| (1,842)  | 1:A:7:LEU:HD11  | 1:A:17:PHE:HD2  | 19       | 0.31          |
| (1,842)  | 1:A:7:LEU:HD12  | 1:A:17:PHE:HD2  | 19       | 0.31          |
| (1,842)  | 1:A:7:LEU:HD13  | 1:A:17:PHE:HD2  | 19       | 0.31          |
| (1,258)  | 1:A:15:PHE:H    | 1:A:33:TYR:HD2  | 2        | 0.31          |
| (1,1822) | 1:A:68:PHE:HE2  | 1:A:81:SER:HB2  | 10       | 0.31          |
| (1,258)  | 1:A:15:PHE:H    | 1:A:33:TYR:HD2  | 18       | 0.3           |
| (1,1807) | 1:A:67:TYR:H    | 1:A:67:TYR:HD2  | 20       | 0.3           |
| (1,1413) | 1:A:68:PHE:HD1  | 1:A:69:ASN:HA   | 10       | 0.3           |
| (1,1398) | 1:A:66:PRO:HG2  | 1:A:84:TYR:HD1  | 13       | 0.3           |
| (1,878)  | 1:A:9:LYS:HB2   | 1:A:15:PHE:HE1  | 3        | 0.29          |
| (1,842)  | 1:A:7:LEU:HD11  | 1:A:17:PHE:HD2  | 1        | 0.29          |
| (1,842)  | 1:A:7:LEU:HD12  | 1:A:17:PHE:HD2  | 1        | 0.29          |
| (1,842)  | 1:A:7:LEU:HD13  | 1:A:17:PHE:HD2  | 1        | 0.29          |
| (1,258)  | 1:A:15:PHE:H    | 1:A:33:TYR:HD2  | 20       | 0.29          |
| (1,1845) | 1:A:82:GLN:H    | 1:A:84:TYR:HE1  | 4        | 0.29          |
| (1,1773) | 1:A:9:LYS:HA    | 1:A:15:PHE:HD1  | 6        | 0.29          |
| (1,887)  | 1:A:9:LYS:HG2   | 1:A:15:PHE:HE1  | 3        | 0.28          |
| (1,470)  | 1:A:68:PHE:HE2  | 1:A:94:ILE:H    | 8        | 0.28          |
| (1,258)  | 1:A:15:PHE:H    | 1:A:33:TYR:HD2  | 9        | 0.28          |
| (1,1836) | 1:A:84:TYR:HA   | 1:A:84:TYR:HD2  | 4        | 0.28          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 9        | 0.28          |
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 13       | 0.28          |
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 20       | 0.28          |
| (1,1799) | 1:A:33:TYR:HE1 | 1:A:42:GLY:HA3  | 18       | 0.28          |
| (1,842)  | 1:A:7:LEU:HD11 | 1:A:17:PHE:HD2  | 2        | 0.27          |
| (1,842)  | 1:A:7:LEU:HD12 | 1:A:17:PHE:HD2  | 2        | 0.27          |
| (1,842)  | 1:A:7:LEU:HD13 | 1:A:17:PHE:HD2  | 2        | 0.27          |
| (1,2261) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HD2  | 9        | 0.27          |
| (1,2261) | 1:A:84:TYR:HE1 | 1:A:90:ARG:HD3  | 9        | 0.27          |
| (1,1908) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HD1  | 5        | 0.27          |
| (1,1908) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HD1  | 5        | 0.27          |
| (1,1885) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HG12 | 17       | 0.27          |
| (1,1885) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HG13 | 17       | 0.27          |
| (1,1845) | 1:A:82:GLN:H   | 1:A:84:TYR:HE1  | 9        | 0.27          |
| (1,1845) | 1:A:82:GLN:H   | 1:A:84:TYR:HE1  | 11       | 0.27          |
| (1,1789) | 1:A:33:TYR:HD1 | 1:A:39:ALA:HA   | 4        | 0.27          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 14       | 0.27          |
| (1,878)  | 1:A:9:LYS:HB2  | 1:A:15:PHE:HE1  | 20       | 0.26          |
| (1,2245) | 1:A:81:SER:HB2 | 1:A:84:TYR:HE1  | 9        | 0.26          |
| (1,2245) | 1:A:81:SER:HB3 | 1:A:84:TYR:HE1  | 9        | 0.26          |
| (1,1917) | 1:A:9:LYS:HG2  | 1:A:15:PHE:HE1  | 12       | 0.26          |
| (1,1917) | 1:A:9:LYS:HG3  | 1:A:15:PHE:HE1  | 12       | 0.26          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG21 | 18       | 0.26          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG22 | 18       | 0.26          |
| (1,1184) | 1:A:17:PHE:HD1 | 1:A:43:ILE:HG23 | 18       | 0.26          |
| (1,842)  | 1:A:7:LEU:HD11 | 1:A:17:PHE:HD2  | 16       | 0.25          |
| (1,842)  | 1:A:7:LEU:HD12 | 1:A:17:PHE:HD2  | 16       | 0.25          |
| (1,842)  | 1:A:7:LEU:HD13 | 1:A:17:PHE:HD2  | 16       | 0.25          |
| (1,1822) | 1:A:68:PHE:HE2 | 1:A:81:SER:HB2  | 7        | 0.25          |
| (1,1773) | 1:A:9:LYS:HA   | 1:A:15:PHE:HD1  | 11       | 0.25          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 6        | 0.25          |
| (1,282)  | 1:A:15:PHE:HD2 | 1:A:36:LYS:H    | 15       | 0.24          |
| (1,1908) | 1:A:9:LYS:HB2  | 1:A:15:PHE:HD1  | 6        | 0.24          |
| (1,1908) | 1:A:9:LYS:HB3  | 1:A:15:PHE:HD1  | 6        | 0.24          |
| (1,1885) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HG12 | 5        | 0.24          |
| (1,1885) | 1:A:5:TYR:HD2  | 1:A:43:ILE:HG13 | 5        | 0.24          |
| (1,1845) | 1:A:82:GLN:H   | 1:A:84:TYR:HE1  | 14       | 0.24          |
| (1,1773) | 1:A:9:LYS:HA   | 1:A:15:PHE:HD1  | 15       | 0.24          |
| (1,258)  | 1:A:15:PHE:H   | 1:A:33:TYR:HD2  | 17       | 0.23          |
| (1,2245) | 1:A:81:SER:HB2 | 1:A:84:TYR:HE1  | 4        | 0.23          |
| (1,2245) | 1:A:81:SER:HB3 | 1:A:84:TYR:HE1  | 4        | 0.23          |
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD2  | 15       | 0.23          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2204) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HD3  | 15       | 0.23          |
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 8        | 0.23          |
| (1,462)  | 1:A:67:TYR:HD2 | 1:A:84:TYR:H    | 5        | 0.22          |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG2  | 12       | 0.22          |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG3  | 12       | 0.22          |
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 11       | 0.22          |
| (1,1799) | 1:A:33:TYR:HE1 | 1:A:42:GLY:HA3  | 14       | 0.22          |
| (1,1326) | 1:A:57:ALA:HB1 | 1:A:71:LYS:HB2  | 5        | 0.22          |
| (1,1326) | 1:A:57:ALA:HB2 | 1:A:71:LYS:HB2  | 5        | 0.22          |
| (1,1326) | 1:A:57:ALA:HB3 | 1:A:71:LYS:HB2  | 5        | 0.22          |
| (1,462)  | 1:A:67:TYR:HD2 | 1:A:84:TYR:H    | 20       | 0.21          |
| (1,258)  | 1:A:15:PHE:H   | 1:A:33:TYR:HD2  | 1        | 0.21          |
| (1,258)  | 1:A:15:PHE:H   | 1:A:33:TYR:HD2  | 3        | 0.21          |
| (1,258)  | 1:A:15:PHE:H   | 1:A:33:TYR:HD2  | 8        | 0.21          |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG2  | 11       | 0.21          |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG3  | 11       | 0.21          |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG11 | 3        | 0.21          |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG12 | 3        | 0.21          |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG13 | 3        | 0.21          |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG21 | 3        | 0.21          |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG22 | 3        | 0.21          |
| (1,2197) | 1:A:68:PHE:HE1 | 1:A:97:VAL:HG23 | 3        | 0.21          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 4        | 0.21          |
| (1,1773) | 1:A:9:LYS:HA   | 1:A:15:PHE:HD1  | 2        | 0.21          |
| (1,470)  | 1:A:68:PHE:HE2 | 1:A:94:ILE:H    | 12       | 0.2           |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG2  | 7        | 0.2           |
| (1,2203) | 1:A:68:PHE:HD2 | 1:A:90:ARG:HG3  | 7        | 0.2           |
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 6        | 0.2           |
| (1,1823) | 1:A:68:PHE:HE2 | 1:A:81:SER:HB3  | 16       | 0.2           |
| (1,1807) | 1:A:67:TYR:H   | 1:A:67:TYR:HD2  | 2        | 0.2           |
| (1,1803) | 1:A:33:TYR:HE1 | 1:A:39:ALA:HA   | 17       | 0.2           |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 1        | 0.2           |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG21 | 5        | 0.2           |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG22 | 5        | 0.2           |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG23 | 5        | 0.2           |
| (1,462)  | 1:A:67:TYR:HD2 | 1:A:84:TYR:H    | 19       | 0.19          |
| (1,258)  | 1:A:15:PHE:H   | 1:A:33:TYR:HD2  | 7        | 0.19          |
| (1,2136) | 1:A:56:TYR:HB2 | 1:A:68:PHE:HD1  | 14       | 0.19          |
| (1,2136) | 1:A:56:TYR:HB3 | 1:A:68:PHE:HD1  | 14       | 0.19          |
| (1,1927) | 1:A:9:LYS:HE2  | 1:A:15:PHE:HE1  | 20       | 0.19          |
| (1,1927) | 1:A:9:LYS:HE3  | 1:A:15:PHE:HE1  | 20       | 0.19          |
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 14       | 0.19          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 18       | 0.19          |
| (1,1823) | 1:A:68:PHE:HE2 | 1:A:81:SER:HB3  | 3        | 0.19          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 17       | 0.19          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 19       | 0.19          |
| (1,1398) | 1:A:66:PRO:HG2 | 1:A:84:TYR:HD1  | 1        | 0.19          |
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 1        | 0.18          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 3        | 0.18          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 11       | 0.18          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 20       | 0.18          |
| (1,1413) | 1:A:68:PHE:HD1 | 1:A:69:ASN:HA   | 7        | 0.18          |
| (1,842)  | 1:A:7:LEU:HD11 | 1:A:17:PHE:HD2  | 4        | 0.17          |
| (1,842)  | 1:A:7:LEU:HD12 | 1:A:17:PHE:HD2  | 4        | 0.17          |
| (1,842)  | 1:A:7:LEU:HD13 | 1:A:17:PHE:HD2  | 4        | 0.17          |
| (1,2235) | 1:A:75:HIS:H   | 1:A:76:GLN:HE21 | 9        | 0.17          |
| (1,2235) | 1:A:75:HIS:H   | 1:A:76:GLN:HE22 | 9        | 0.17          |
| (1,1836) | 1:A:84:TYR:HA  | 1:A:84:TYR:HD2  | 15       | 0.17          |
| (1,1799) | 1:A:33:TYR:HE1 | 1:A:42:GLY:HA3  | 1        | 0.17          |
| (1,1797) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HE1  | 4        | 0.17          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 2        | 0.17          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 5        | 0.17          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 7        | 0.17          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 8        | 0.17          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 9        | 0.17          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 10       | 0.17          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 13       | 0.17          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG21 | 12       | 0.17          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG22 | 12       | 0.17          |
| (1,1591) | 1:A:68:PHE:HD1 | 1:A:94:ILE:HG23 | 12       | 0.17          |
| (1,1398) | 1:A:66:PRO:HG2 | 1:A:84:TYR:HD1  | 3        | 0.17          |
| (1,987)  | 1:A:21:ALA:HB1 | 1:A:22:GLY:H    | 20       | 0.16          |
| (1,987)  | 1:A:21:ALA:HB2 | 1:A:22:GLY:H    | 20       | 0.16          |
| (1,987)  | 1:A:21:ALA:HB3 | 1:A:22:GLY:H    | 20       | 0.16          |
| (1,887)  | 1:A:9:LYS:HG2  | 1:A:15:PHE:HE1  | 2        | 0.16          |
| (1,842)  | 1:A:7:LEU:HD11 | 1:A:17:PHE:HD2  | 7        | 0.16          |
| (1,842)  | 1:A:7:LEU:HD12 | 1:A:17:PHE:HD2  | 7        | 0.16          |
| (1,842)  | 1:A:7:LEU:HD13 | 1:A:17:PHE:HD2  | 7        | 0.16          |
| (1,470)  | 1:A:68:PHE:HE2 | 1:A:94:ILE:H    | 9        | 0.16          |
| (1,2235) | 1:A:75:HIS:H   | 1:A:76:GLN:HE21 | 14       | 0.16          |
| (1,2235) | 1:A:75:HIS:H   | 1:A:76:GLN:HE22 | 14       | 0.16          |
| (1,1797) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HE1  | 1        | 0.16          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 6        | 0.16          |
| (1,1787) | 1:A:33:TYR:HB3 | 1:A:33:TYR:HD1  | 12       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1787) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HD1  | 14       | 0.16          |
| (1,1787) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HD1  | 15       | 0.16          |
| (1,1787) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HD1  | 16       | 0.16          |
| (1,1409) | 1:A:67:TYR:HD1  | 1:A:68:PHE:HA   | 7        | 0.16          |
| (1,987)  | 1:A:21:ALA:HB1  | 1:A:22:GLY:H    | 7        | 0.15          |
| (1,987)  | 1:A:21:ALA:HB2  | 1:A:22:GLY:H    | 7        | 0.15          |
| (1,987)  | 1:A:21:ALA:HB3  | 1:A:22:GLY:H    | 7        | 0.15          |
| (1,887)  | 1:A:9:LYS:HG2   | 1:A:15:PHE:HE1  | 15       | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 2        | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 2        | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 5        | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 5        | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 7        | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 7        | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 12       | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 12       | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 13       | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 13       | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 16       | 0.15          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 16       | 0.15          |
| (1,2202) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB2  | 17       | 0.15          |
| (1,2202) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB3  | 17       | 0.15          |
| (1,1908) | 1:A:9:LYS:HB2   | 1:A:15:PHE:HD1  | 11       | 0.15          |
| (1,1908) | 1:A:9:LYS:HB3   | 1:A:15:PHE:HD1  | 11       | 0.15          |
| (1,1845) | 1:A:82:GLN:H    | 1:A:84:TYR:HE1  | 15       | 0.15          |
| (1,1840) | 1:A:84:TYR:HD1  | 1:A:90:ARG:HA   | 15       | 0.15          |
| (1,1828) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB2  | 15       | 0.15          |
| (1,1799) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA3  | 16       | 0.15          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 11       | 0.15          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 17       | 0.15          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 19       | 0.15          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2  | 18       | 0.15          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG21 | 2        | 0.15          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG22 | 2        | 0.15          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG23 | 2        | 0.15          |
| (1,1497) | 1:A:27:ILE:HD11 | 1:A:97:VAL:HB   | 2        | 0.15          |
| (1,1497) | 1:A:27:ILE:HD12 | 1:A:97:VAL:HB   | 2        | 0.15          |
| (1,1497) | 1:A:27:ILE:HD13 | 1:A:97:VAL:HB   | 2        | 0.15          |
| (1,1497) | 1:A:27:ILE:HD11 | 1:A:97:VAL:HB   | 11       | 0.15          |
| (1,1497) | 1:A:27:ILE:HD12 | 1:A:97:VAL:HB   | 11       | 0.15          |
| (1,1497) | 1:A:27:ILE:HD13 | 1:A:97:VAL:HB   | 11       | 0.15          |
| (1,1497) | 1:A:27:ILE:HD11 | 1:A:97:VAL:HB   | 14       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1497) | 1:A:27:ILE:HD12 | 1:A:97:VAL:HB   | 14       | 0.15          |
| (1,1497) | 1:A:27:ILE:HD13 | 1:A:97:VAL:HB   | 14       | 0.15          |
| (1,1058) | 1:A:28:LEU:HD11 | 1:A:68:PHE:HD1  | 17       | 0.15          |
| (1,1058) | 1:A:28:LEU:HD12 | 1:A:68:PHE:HD1  | 17       | 0.15          |
| (1,1058) | 1:A:28:LEU:HD13 | 1:A:68:PHE:HD1  | 17       | 0.15          |
| (1,850)  | 1:A:7:LEU:HD21  | 1:A:8:SER:HA    | 7        | 0.14          |
| (1,850)  | 1:A:7:LEU:HD22  | 1:A:8:SER:HA    | 7        | 0.14          |
| (1,850)  | 1:A:7:LEU:HD23  | 1:A:8:SER:HA    | 7        | 0.14          |
| (1,850)  | 1:A:7:LEU:HD21  | 1:A:8:SER:HA    | 18       | 0.14          |
| (1,850)  | 1:A:7:LEU:HD22  | 1:A:8:SER:HA    | 18       | 0.14          |
| (1,850)  | 1:A:7:LEU:HD23  | 1:A:8:SER:HA    | 18       | 0.14          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 11       | 0.14          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 11       | 0.14          |
| (1,2185) | 1:A:65:LYS:HD2  | 1:A:83:MET:HB2  | 19       | 0.14          |
| (1,2185) | 1:A:65:LYS:HD2  | 1:A:83:MET:HB3  | 19       | 0.14          |
| (1,2185) | 1:A:65:LYS:HD3  | 1:A:83:MET:HB2  | 19       | 0.14          |
| (1,2185) | 1:A:65:LYS:HD3  | 1:A:83:MET:HB3  | 19       | 0.14          |
| (1,1823) | 1:A:68:PHE:HE2  | 1:A:81:SER:HB3  | 20       | 0.14          |
| (1,1801) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA2  | 8        | 0.14          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 3        | 0.14          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 8        | 0.14          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 9        | 0.14          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 10       | 0.14          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 13       | 0.14          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 14       | 0.14          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 20       | 0.14          |
| (1,1787) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HD1  | 18       | 0.14          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG21 | 1        | 0.14          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG22 | 1        | 0.14          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG23 | 1        | 0.14          |
| (1,1497) | 1:A:27:ILE:HD11 | 1:A:97:VAL:HB   | 7        | 0.14          |
| (1,1497) | 1:A:27:ILE:HD12 | 1:A:97:VAL:HB   | 7        | 0.14          |
| (1,1497) | 1:A:27:ILE:HD13 | 1:A:97:VAL:HB   | 7        | 0.14          |
| (1,1497) | 1:A:27:ILE:HD11 | 1:A:97:VAL:HB   | 10       | 0.14          |
| (1,1497) | 1:A:27:ILE:HD12 | 1:A:97:VAL:HB   | 10       | 0.14          |
| (1,1497) | 1:A:27:ILE:HD13 | 1:A:97:VAL:HB   | 10       | 0.14          |
| (1,987)  | 1:A:21:ALA:HB1  | 1:A:22:GLY:H    | 18       | 0.13          |
| (1,987)  | 1:A:21:ALA:HB2  | 1:A:22:GLY:H    | 18       | 0.13          |
| (1,987)  | 1:A:21:ALA:HB3  | 1:A:22:GLY:H    | 18       | 0.13          |
| (1,850)  | 1:A:7:LEU:HD21  | 1:A:8:SER:HA    | 17       | 0.13          |
| (1,850)  | 1:A:7:LEU:HD22  | 1:A:8:SER:HA    | 17       | 0.13          |
| (1,850)  | 1:A:7:LEU:HD23  | 1:A:8:SER:HA    | 17       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,595)  | 1:A:84:TYR:H    | 1:A:84:TYR:HD1  | 10       | 0.13          |
| (1,470)  | 1:A:68:PHE:HE2  | 1:A:94:ILE:H    | 4        | 0.13          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 3        | 0.13          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 3        | 0.13          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 17       | 0.13          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 17       | 0.13          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 20       | 0.13          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 20       | 0.13          |
| (1,2185) | 1:A:65:LYS:HD2  | 1:A:83:MET:HB2  | 3        | 0.13          |
| (1,2185) | 1:A:65:LYS:HD2  | 1:A:83:MET:HB3  | 3        | 0.13          |
| (1,2185) | 1:A:65:LYS:HD3  | 1:A:83:MET:HB2  | 3        | 0.13          |
| (1,2185) | 1:A:65:LYS:HD3  | 1:A:83:MET:HB3  | 3        | 0.13          |
| (1,1836) | 1:A:84:TYR:HA   | 1:A:84:TYR:HD2  | 3        | 0.13          |
| (1,1836) | 1:A:84:TYR:HA   | 1:A:84:TYR:HD2  | 12       | 0.13          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 2        | 0.13          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 5        | 0.13          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 6        | 0.13          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 7        | 0.13          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 12       | 0.13          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 15       | 0.13          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1  | 16       | 0.13          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2  | 6        | 0.13          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2  | 10       | 0.13          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2  | 12       | 0.13          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2  | 15       | 0.13          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2  | 16       | 0.13          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG21 | 11       | 0.13          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG22 | 11       | 0.13          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG23 | 11       | 0.13          |
| (1,1497) | 1:A:27:ILE:HD11 | 1:A:97:VAL:HB   | 13       | 0.13          |
| (1,1497) | 1:A:27:ILE:HD12 | 1:A:97:VAL:HB   | 13       | 0.13          |
| (1,1497) | 1:A:27:ILE:HD13 | 1:A:97:VAL:HB   | 13       | 0.13          |
| (1,1413) | 1:A:68:PHE:HD1  | 1:A:69:ASN:HA   | 19       | 0.13          |
| (1,898)  | 1:A:12:ASN:HB3  | 1:A:14:GLN:HG2  | 13       | 0.12          |
| (1,887)  | 1:A:9:LYS:HG2   | 1:A:15:PHE:HE1  | 11       | 0.12          |
| (1,850)  | 1:A:7:LEU:HD21  | 1:A:8:SER:HA    | 3        | 0.12          |
| (1,850)  | 1:A:7:LEU:HD22  | 1:A:8:SER:HA    | 3        | 0.12          |
| (1,850)  | 1:A:7:LEU:HD23  | 1:A:8:SER:HA    | 3        | 0.12          |
| (1,850)  | 1:A:7:LEU:HD21  | 1:A:8:SER:HA    | 10       | 0.12          |
| (1,850)  | 1:A:7:LEU:HD22  | 1:A:8:SER:HA    | 10       | 0.12          |
| (1,850)  | 1:A:7:LEU:HD23  | 1:A:8:SER:HA    | 10       | 0.12          |
| (1,523)  | 1:A:55:ARG:HE   | 1:A:73:ALA:HB1  | 16       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,523)  | 1:A:55:ARG:HE   | 1:A:73:ALA:HB2  | 16       | 0.12          |
| (1,523)  | 1:A:55:ARG:HE   | 1:A:73:ALA:HB3  | 16       | 0.12          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 1        | 0.12          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 1        | 0.12          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 10       | 0.12          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 10       | 0.12          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 18       | 0.12          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 18       | 0.12          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG2  | 6        | 0.12          |
| (1,2203) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HG3  | 6        | 0.12          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG11 | 15       | 0.12          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG12 | 15       | 0.12          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG13 | 15       | 0.12          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG21 | 15       | 0.12          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG22 | 15       | 0.12          |
| (1,2197) | 1:A:68:PHE:HE1  | 1:A:97:VAL:HG23 | 15       | 0.12          |
| (1,1845) | 1:A:82:GLN:H    | 1:A:84:TYR:HE1  | 12       | 0.12          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2  | 2        | 0.12          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2  | 3        | 0.12          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2  | 5        | 0.12          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2  | 7        | 0.12          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2  | 14       | 0.12          |
| (1,163)  | 1:A:20:LYS:HB3  | 1:A:21:ALA:H    | 12       | 0.12          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG21 | 14       | 0.12          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG22 | 14       | 0.12          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG23 | 14       | 0.12          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG21 | 15       | 0.12          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG22 | 15       | 0.12          |
| (1,1591) | 1:A:68:PHE:HD1  | 1:A:94:ILE:HG23 | 15       | 0.12          |
| (1,850)  | 1:A:7:LEU:HD21  | 1:A:8:SER:HA    | 14       | 0.11          |
| (1,850)  | 1:A:7:LEU:HD22  | 1:A:8:SER:HA    | 14       | 0.11          |
| (1,850)  | 1:A:7:LEU:HD23  | 1:A:8:SER:HA    | 14       | 0.11          |
| (1,850)  | 1:A:7:LEU:HD21  | 1:A:8:SER:HA    | 16       | 0.11          |
| (1,850)  | 1:A:7:LEU:HD22  | 1:A:8:SER:HA    | 16       | 0.11          |
| (1,850)  | 1:A:7:LEU:HD23  | 1:A:8:SER:HA    | 16       | 0.11          |
| (1,448)  | 1:A:63:ASN:HD22 | 1:A:65:LYS:HD3  | 17       | 0.11          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 6        | 0.11          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 6        | 0.11          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 8        | 0.11          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 8        | 0.11          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE21 | 15       | 0.11          |
| (1,2235) | 1:A:75:HIS:H    | 1:A:76:GLN:HE22 | 15       | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD2   | 5        | 0.11          |
| (1,2204) | 1:A:68:PHE:HD2  | 1:A:90:ARG:HD3   | 5        | 0.11          |
| (1,2055) | 1:A:38:GLY:HA2  | 1:A:41:ASN:HD21  | 16       | 0.11          |
| (1,2055) | 1:A:38:GLY:HA2  | 1:A:41:ASN:HD22  | 16       | 0.11          |
| (1,2017) | 1:A:27:ILE:HG21 | 1:A:97:VAL:HG11  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG21 | 1:A:97:VAL:HG12  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG21 | 1:A:97:VAL:HG13  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG21 | 1:A:97:VAL:HG21  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG21 | 1:A:97:VAL:HG22  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG21 | 1:A:97:VAL:HG23  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG22 | 1:A:97:VAL:HG11  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG22 | 1:A:97:VAL:HG12  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG22 | 1:A:97:VAL:HG13  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG22 | 1:A:97:VAL:HG21  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG22 | 1:A:97:VAL:HG22  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG22 | 1:A:97:VAL:HG23  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG23 | 1:A:97:VAL:HG11  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG23 | 1:A:97:VAL:HG12  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG23 | 1:A:97:VAL:HG13  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG23 | 1:A:97:VAL:HG21  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG23 | 1:A:97:VAL:HG22  | 8        | 0.11          |
| (1,2017) | 1:A:27:ILE:HG23 | 1:A:97:VAL:HG23  | 8        | 0.11          |
| (1,1927) | 1:A:9:LYS:HE2   | 1:A:15:PHE:HE1   | 11       | 0.11          |
| (1,1927) | 1:A:9:LYS:HE3   | 1:A:15:PHE:HE1   | 11       | 0.11          |
| (1,1886) | 1:A:5:TYR:HD2   | 1:A:106:ILE:HG12 | 9        | 0.11          |
| (1,1886) | 1:A:5:TYR:HD2   | 1:A:106:ILE:HG13 | 9        | 0.11          |
| (1,1845) | 1:A:82:GLN:H    | 1:A:84:TYR:HE1   | 13       | 0.11          |
| (1,1828) | 1:A:68:PHE:HD2  | 1:A:81:SER:HB2   | 2        | 0.11          |
| (1,1801) | 1:A:33:TYR:HE1  | 1:A:42:GLY:HA2   | 6        | 0.11          |
| (1,1797) | 1:A:33:TYR:HB3  | 1:A:33:TYR:HE1   | 18       | 0.11          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2   | 8        | 0.11          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2   | 9        | 0.11          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2   | 11       | 0.11          |
| (1,1788) | 1:A:33:TYR:HB2  | 1:A:33:TYR:HD2   | 13       | 0.11          |
| (1,155)  | 1:A:4:TRP:H     | 1:A:20:LYS:HB2   | 12       | 0.11          |
| (1,1497) | 1:A:27:ILE:HD11 | 1:A:97:VAL:HB    | 1        | 0.11          |
| (1,1497) | 1:A:27:ILE:HD12 | 1:A:97:VAL:HB    | 1        | 0.11          |
| (1,1497) | 1:A:27:ILE:HD13 | 1:A:97:VAL:HB    | 1        | 0.11          |
| (1,1497) | 1:A:27:ILE:HD11 | 1:A:97:VAL:HB    | 16       | 0.11          |
| (1,1497) | 1:A:27:ILE:HD12 | 1:A:97:VAL:HB    | 16       | 0.11          |
| (1,1497) | 1:A:27:ILE:HD13 | 1:A:97:VAL:HB    | 16       | 0.11          |
| (1,1497) | 1:A:27:ILE:HD11 | 1:A:97:VAL:HB    | 20       | 0.11          |

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| <b>Key</b> | <b>Atom-1</b>   | <b>Atom-2</b>   | <b>Model ID</b> | <b>Violation (Å)</b> |
|------------|-----------------|-----------------|-----------------|----------------------|
| (1,1497)   | 1:A:27:ILE:HD12 | 1:A:97:VAL:HB   | 20              | 0.11                 |
| (1,1497)   | 1:A:27:ILE:HD13 | 1:A:97:VAL:HB   | 20              | 0.11                 |
| (1,1413)   | 1:A:68:PHE:HD1  | 1:A:69:ASN:HA   | 17              | 0.11                 |
| (1,1324)   | 1:A:57:ALA:HB1  | 1:A:69:ASN:HB3  | 7               | 0.11                 |
| (1,1324)   | 1:A:57:ALA:HB2  | 1:A:69:ASN:HB3  | 7               | 0.11                 |
| (1,1324)   | 1:A:57:ALA:HB3  | 1:A:69:ASN:HB3  | 7               | 0.11                 |
| (1,1050)   | 1:A:28:LEU:HB2  | 1:A:97:VAL:HG11 | 9               | 0.11                 |
| (1,1050)   | 1:A:28:LEU:HB2  | 1:A:97:VAL:HG12 | 9               | 0.11                 |
| (1,1050)   | 1:A:28:LEU:HB2  | 1:A:97:VAL:HG13 | 9               | 0.11                 |

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

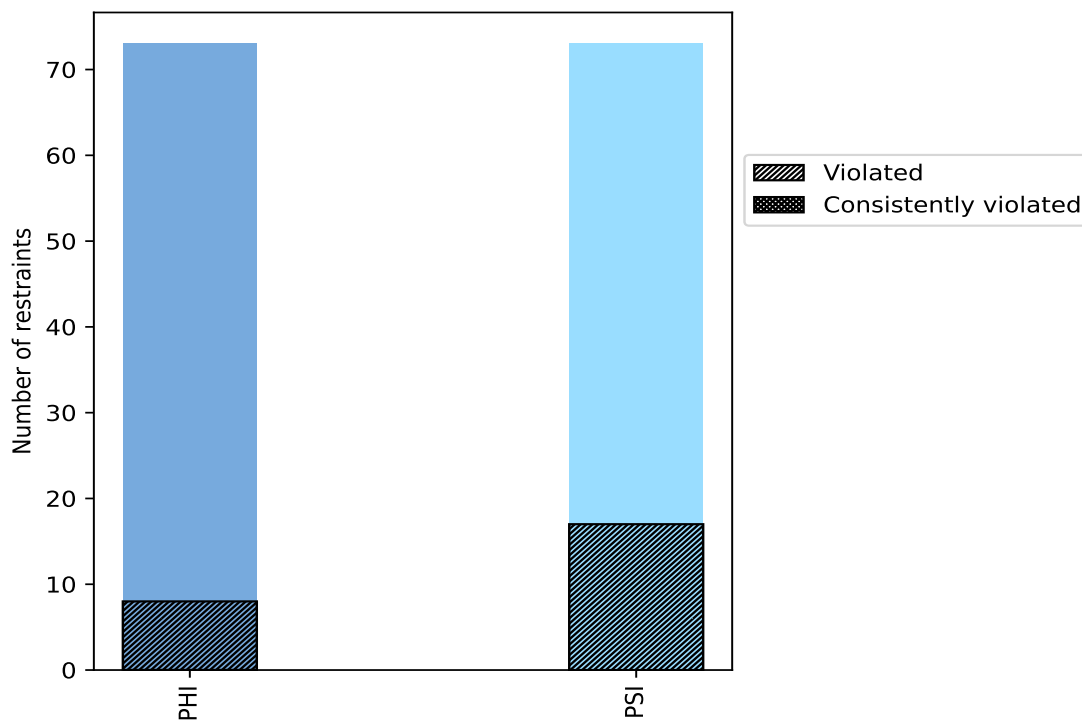
### 10.1 Summary of dihedral-angle violations [i](#)

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> |
| PHI        | 73    | 50.0           | 8                     | 11.0           | 5.5            | 0                                  | 0.0            | 0.0            |
| PSI        | 73    | 50.0           | 17                    | 23.3           | 11.6           | 0                                  | 0.0            | 0.0            |
| Total      | 146   | 100.0          | 25                    | 17.1           | 17.1           | 0                                  | 0.0            | 0.0            |

<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

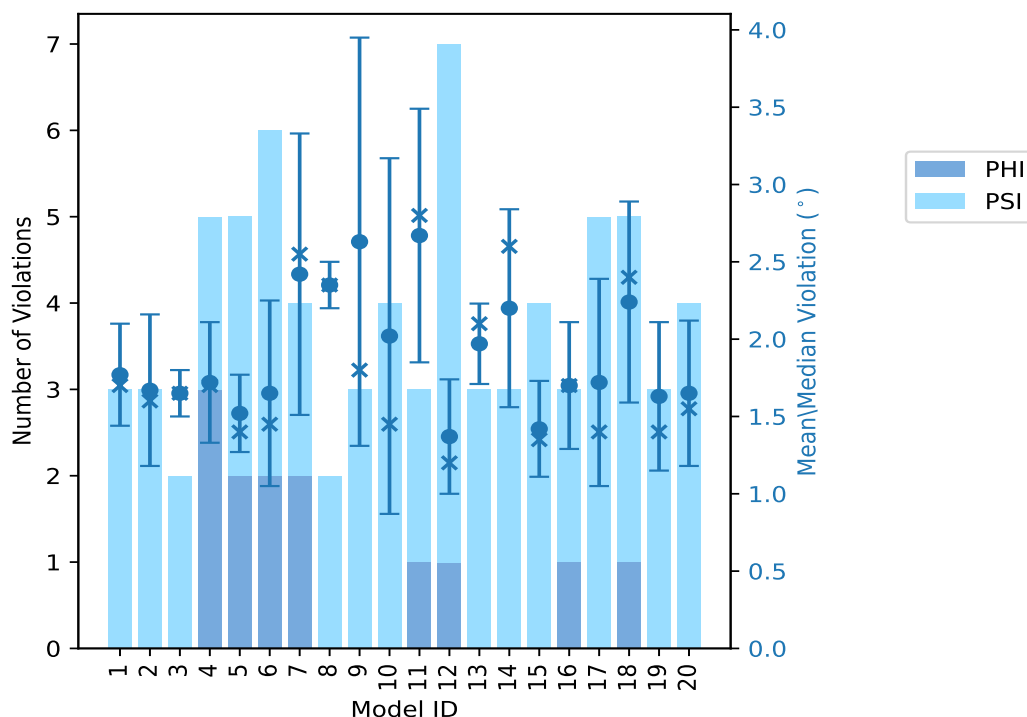


## 10.2 Dihedral-angle violation statistics for each model [i](#)

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 (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 0                    | 3   | 3     | 1.77     | 2.2     | 0.33   | 1.7        |
| 2        | 0                    | 3   | 3     | 1.67     | 2.3     | 0.49   | 1.6        |
| 3        | 0                    | 2   | 2     | 1.65     | 1.8     | 0.15   | 1.65       |
| 4        | 3                    | 2   | 5     | 1.72     | 2.4     | 0.39   | 1.7        |
| 5        | 2                    | 3   | 5     | 1.52     | 2.0     | 0.25   | 1.4        |
| 6        | 2                    | 4   | 6     | 1.65     | 2.8     | 0.6    | 1.45       |
| 7        | 2                    | 2   | 4     | 2.42     | 3.4     | 0.91   | 2.55       |
| 8        | 0                    | 2   | 2     | 2.35     | 2.5     | 0.15   | 2.35       |
| 9        | 0                    | 3   | 3     | 2.63     | 4.5     | 1.32   | 1.8        |
| 10       | 0                    | 4   | 4     | 2.02     | 4.0     | 1.15   | 1.45       |
| 11       | 1                    | 2   | 3     | 2.67     | 3.6     | 0.82   | 2.8        |
| 12       | 1                    | 6   | 7     | 1.37     | 2.0     | 0.37   | 1.2        |
| 13       | 0                    | 3   | 3     | 1.97     | 2.2     | 0.26   | 2.1        |
| 14       | 0                    | 3   | 3     | 2.2      | 2.7     | 0.64   | 2.6        |
| 15       | 0                    | 4   | 4     | 1.42     | 1.9     | 0.31   | 1.35       |
| 16       | 1                    | 2   | 3     | 1.7      | 2.2     | 0.41   | 1.7        |
| 17       | 0                    | 5   | 5     | 1.72     | 3.0     | 0.67   | 1.4        |
| 18       | 1                    | 4   | 5     | 2.24     | 3.1     | 0.65   | 2.4        |
| 19       | 0                    | 3   | 3     | 1.63     | 2.3     | 0.48   | 1.4        |
| 20       | 0                    | 4   | 4     | 1.65     | 2.4     | 0.47   | 1.55       |

### 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 |      |
|-------------------------------|-----|-------|--------------------------|------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %    |
| 5                             | 9   | 14    | 1                        | 5.0  |
| 1                             | 2   | 3     | 2                        | 10.0 |
| 2                             | 1   | 3     | 3                        | 15.0 |
| 0                             | 0   | 0     | 4                        | 20.0 |
| 0                             | 1   | 1     | 5                        | 25.0 |
| 0                             | 1   | 1     | 6                        | 30.0 |
| 0                             | 1   | 1     | 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 |

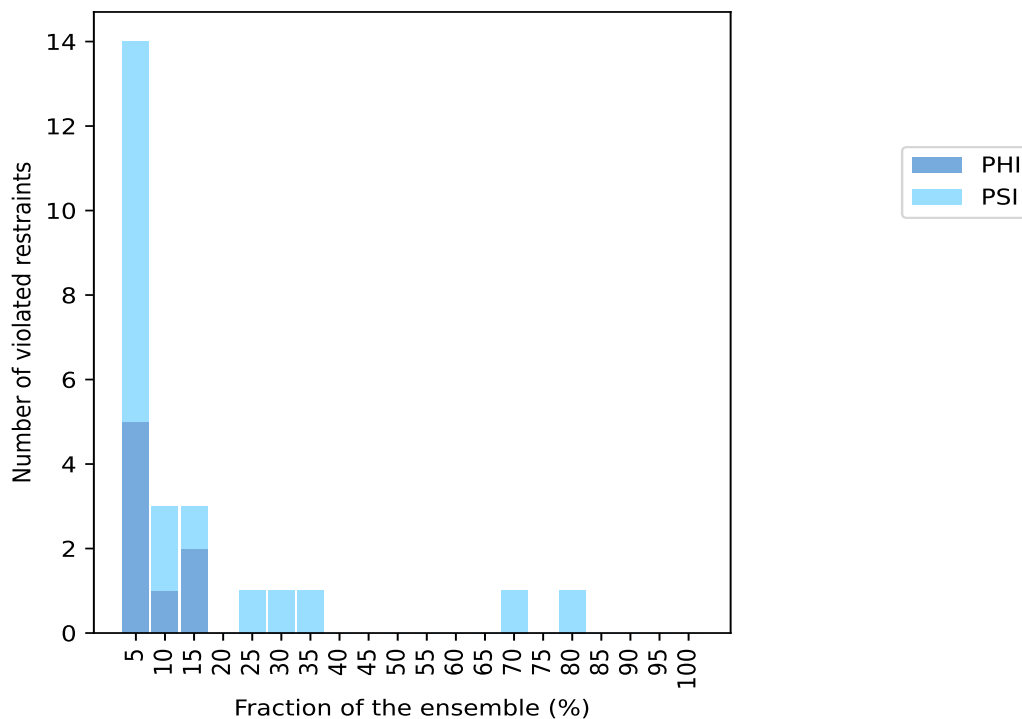
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |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

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

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

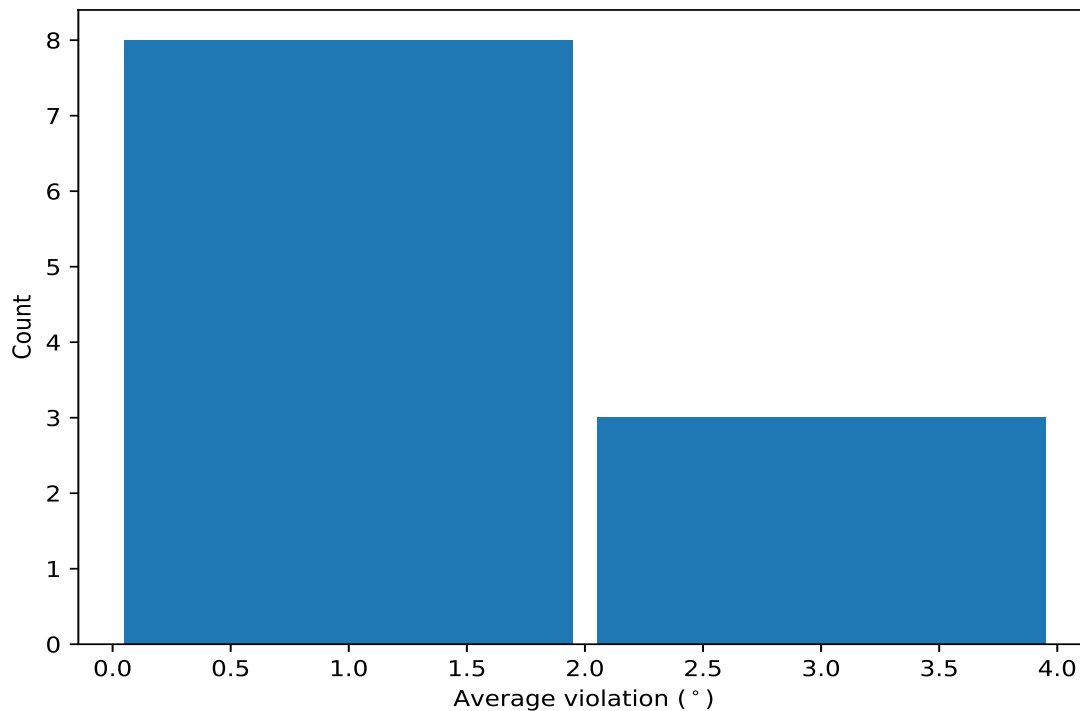


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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.

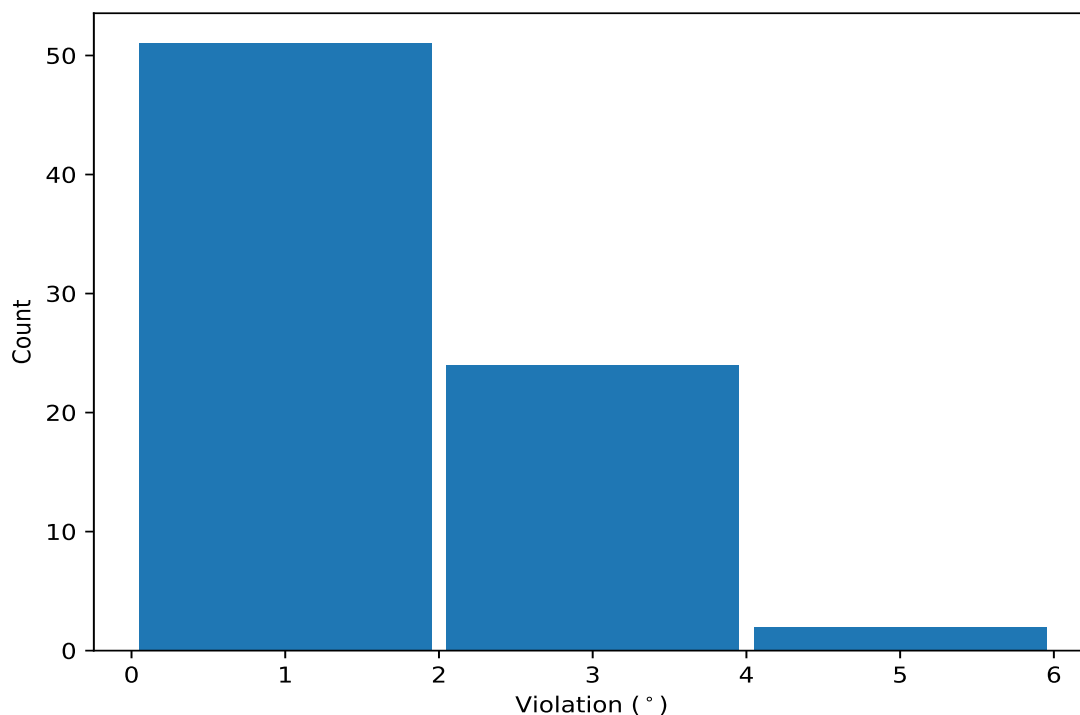
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,102) | 1:A:72:ALA:N | 1:A:72:ALA:CA | 1:A:72:ALA:C  | 1:A:73:ALA:N | 16                  | 2.19 | 0.69            | 1.95   |
| (1,68)  | 1:A:49:ASN:N | 1:A:49:ASN:CA | 1:A:49:ASN:C  | 1:A:50:SER:N | 14                  | 2.44 | 0.94            | 2.3    |
| (1,92)  | 1:A:67:TYR:N | 1:A:67:TYR:CA | 1:A:67:TYR:C  | 1:A:68:PHE:N | 7                   | 1.66 | 0.4             | 1.5    |
| (1,76)  | 1:A:57:ALA:N | 1:A:57:ALA:CA | 1:A:57:ALA:C  | 1:A:58:LYS:N | 6                   | 2.03 | 0.48            | 1.75   |
| (1,136) | 1:A:98:MET:N | 1:A:98:MET:CA | 1:A:98:MET:C  | 1:A:99:GLU:N | 5                   | 1.44 | 0.45            | 1.3    |
| (1,78)  | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C  | 1:A:59:GLU:N | 3                   | 1.8  | 0.59            | 1.6    |
| (1,31)  | 1:A:27:ILE:C | 1:A:28:LEU:N  | 1:A:28:LEU:CA | 1:A:28:LEU:C | 3                   | 1.63 | 0.21            | 1.6    |
| (1,97)  | 1:A:69:ASN:C | 1:A:70:LEU:N  | 1:A:70:LEU:CA | 1:A:70:LEU:C | 3                   | 1.33 | 0.19            | 1.2    |
| (1,28)  | 1:A:23:ASN:N | 1:A:23:ASN:CA | 1:A:23:ASN:C  | 1:A:24:GLY:N | 2                   | 1.45 | 0.05            | 1.45   |
| (1,114) | 1:A:87:THR:N | 1:A:87:THR:CA | 1:A:87:THR:C  | 1:A:88:ALA:N | 2                   | 1.35 | 0.15            | 1.35   |
| (1,21)  | 1:A:17:PHE:C | 1:A:18:VAL:N  | 1:A:18:VAL:CA | 1:A:18:VAL:C | 2                   | 1.25 | 0.15            | 1.25   |

<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 (°) |
|---------|--------------|---------------|--------------|--------------|----------|---------------|
| (1,68)  | 1:A:49:ASN:N | 1:A:49:ASN:CA | 1:A:49:ASN:C | 1:A:50:SER:N | 9        | 4.5           |
| (1,102) | 1:A:72:ALA:N | 1:A:72:ALA:CA | 1:A:72:ALA:C | 1:A:73:ALA:N | 10       | 4.0           |
| (1,68)  | 1:A:49:ASN:N | 1:A:49:ASN:CA | 1:A:49:ASN:C | 1:A:50:SER:N | 11       | 3.6           |
| (1,102) | 1:A:72:ALA:N | 1:A:72:ALA:CA | 1:A:72:ALA:C | 1:A:73:ALA:N | 7        | 3.4           |
| (1,68)  | 1:A:49:ASN:N | 1:A:49:ASN:CA | 1:A:49:ASN:C | 1:A:50:SER:N | 7        | 3.2           |
| (1,68)  | 1:A:49:ASN:N | 1:A:49:ASN:CA | 1:A:49:ASN:C | 1:A:50:SER:N | 18       | 3.1           |
| (1,68)  | 1:A:49:ASN:N | 1:A:49:ASN:CA | 1:A:49:ASN:C | 1:A:50:SER:N | 17       | 3.0           |
| (1,76)  | 1:A:57:ALA:N | 1:A:57:ALA:CA | 1:A:57:ALA:C | 1:A:58:LYS:N | 6        | 2.8           |
| (1,102) | 1:A:72:ALA:N | 1:A:72:ALA:CA | 1:A:72:ALA:C | 1:A:73:ALA:N | 11       | 2.8           |
| (1,68)  | 1:A:49:ASN:N | 1:A:49:ASN:CA | 1:A:49:ASN:C | 1:A:50:SER:N | 14       | 2.7           |
| (1,78)  | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 1:A:59:GLU:N | 14       | 2.6           |
| (1,76)  | 1:A:57:ALA:N | 1:A:57:ALA:CA | 1:A:57:ALA:C | 1:A:58:LYS:N | 18       | 2.6           |
| (1,102) | 1:A:72:ALA:N | 1:A:72:ALA:CA | 1:A:72:ALA:C | 1:A:73:ALA:N | 8        | 2.5           |
| (1,68)  | 1:A:49:ASN:N | 1:A:49:ASN:CA | 1:A:49:ASN:C | 1:A:50:SER:N | 4        | 2.4           |

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| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,27)  | 1:A:22:GLY:C  | 1:A:23:ASN:N   | 1:A:23:ASN:CA | 1:A:23:ASN:C  | 18       | 2.4           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 20       | 2.4           |
| (1,136) | 1:A:98:MET:N  | 1:A:98:MET:CA  | 1:A:98:MET:C  | 1:A:99:GLU:N  | 2        | 2.3           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 19       | 2.3           |
| (1,92)  | 1:A:67:TYR:N  | 1:A:67:TYR:CA  | 1:A:67:TYR:C  | 1:A:68:PHE:N  | 8        | 2.2           |
| (1,92)  | 1:A:67:TYR:N  | 1:A:67:TYR:CA  | 1:A:67:TYR:C  | 1:A:68:PHE:N  | 16       | 2.2           |
| (1,68)  | 1:A:49:ASN:N  | 1:A:49:ASN:CA  | 1:A:49:ASN:C  | 1:A:50:SER:N  | 1        | 2.2           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 13       | 2.2           |
| (1,68)  | 1:A:49:ASN:N  | 1:A:49:ASN:CA  | 1:A:49:ASN:C  | 1:A:50:SER:N  | 13       | 2.1           |
| (1,68)  | 1:A:49:ASN:N  | 1:A:49:ASN:CA  | 1:A:49:ASN:C  | 1:A:50:SER:N  | 6        | 2.0           |
| (1,142) | 1:A:106:ILE:N | 1:A:106:ILE:CA | 1:A:106:ILE:C | 1:A:107:LYS:N | 12       | 2.0           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 5        | 2.0           |
| (1,31)  | 1:A:27:ILE:C  | 1:A:28:LEU:N   | 1:A:28:LEU:CA | 1:A:28:LEU:C  | 7        | 1.9           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 12       | 1.9           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 15       | 1.9           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 18       | 1.9           |
| (1,92)  | 1:A:67:TYR:N  | 1:A:67:TYR:CA  | 1:A:67:TYR:C  | 1:A:68:PHE:N  | 9        | 1.8           |
| (1,76)  | 1:A:57:ALA:N  | 1:A:57:ALA:CA  | 1:A:57:ALA:C  | 1:A:58:LYS:N  | 3        | 1.8           |
| (1,76)  | 1:A:57:ALA:N  | 1:A:57:ALA:CA  | 1:A:57:ALA:C  | 1:A:58:LYS:N  | 1        | 1.7           |
| (1,76)  | 1:A:57:ALA:N  | 1:A:57:ALA:CA  | 1:A:57:ALA:C  | 1:A:58:LYS:N  | 17       | 1.7           |
| (1,68)  | 1:A:49:ASN:N  | 1:A:49:ASN:CA  | 1:A:49:ASN:C  | 1:A:50:SER:N  | 16       | 1.7           |
| (1,107) | 1:A:75:HIS:C  | 1:A:76:GLN:N   | 1:A:76:GLN:CA | 1:A:76:GLN:C  | 4        | 1.7           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 4        | 1.7           |
| (1,97)  | 1:A:69:ASN:C  | 1:A:70:LEU:N   | 1:A:70:LEU:CA | 1:A:70:LEU:C  | 11       | 1.6           |
| (1,78)  | 1:A:58:LYS:N  | 1:A:58:LYS:CA  | 1:A:58:LYS:C  | 1:A:59:GLU:N  | 20       | 1.6           |
| (1,76)  | 1:A:57:ALA:N  | 1:A:57:ALA:CA  | 1:A:57:ALA:C  | 1:A:58:LYS:N  | 10       | 1.6           |
| (1,31)  | 1:A:27:ILE:C  | 1:A:28:LEU:N   | 1:A:28:LEU:CA | 1:A:28:LEU:C  | 4        | 1.6           |
| (1,120) | 1:A:90:ARG:N  | 1:A:90:ARG:CA  | 1:A:90:ARG:C  | 1:A:91:ASP:N  | 13       | 1.6           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 2        | 1.6           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 9        | 1.6           |
| (1,92)  | 1:A:67:TYR:N  | 1:A:67:TYR:CA  | 1:A:67:TYR:C  | 1:A:68:PHE:N  | 15       | 1.5           |
| (1,92)  | 1:A:67:TYR:N  | 1:A:67:TYR:CA  | 1:A:67:TYR:C  | 1:A:68:PHE:N  | 20       | 1.5           |
| (1,28)  | 1:A:23:ASN:N  | 1:A:23:ASN:CA  | 1:A:23:ASN:C  | 1:A:24:GLY:N  | 6        | 1.5           |
| (1,114) | 1:A:87:THR:N  | 1:A:87:THR:CA  | 1:A:87:THR:C  | 1:A:88:ALA:N  | 5        | 1.5           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 3        | 1.5           |
| (1,8)   | 1:A:8:SER:N   | 1:A:8:SER:CA   | 1:A:8:SER:C   | 1:A:9:LYS:N   | 17       | 1.4           |
| (1,68)  | 1:A:49:ASN:N  | 1:A:49:ASN:CA  | 1:A:49:ASN:C  | 1:A:50:SER:N  | 19       | 1.4           |
| (1,31)  | 1:A:27:ILE:C  | 1:A:28:LEU:N   | 1:A:28:LEU:CA | 1:A:28:LEU:C  | 6        | 1.4           |
| (1,28)  | 1:A:23:ASN:N  | 1:A:23:ASN:CA  | 1:A:23:ASN:C  | 1:A:24:GLY:N  | 17       | 1.4           |
| (1,21)  | 1:A:17:PHE:C  | 1:A:18:VAL:N   | 1:A:18:VAL:CA | 1:A:18:VAL:C  | 5        | 1.4           |
| (1,136) | 1:A:98:MET:N  | 1:A:98:MET:CA  | 1:A:98:MET:C  | 1:A:99:GLU:N  | 5        | 1.4           |
| (1,102) | 1:A:72:ALA:N  | 1:A:72:ALA:CA  | 1:A:72:ALA:C  | 1:A:73:ALA:N  | 1        | 1.4           |
| (1,92)  | 1:A:67:TYR:N  | 1:A:67:TYR:CA  | 1:A:67:TYR:C  | 1:A:68:PHE:N  | 14       | 1.3           |
| (1,136) | 1:A:98:MET:N  | 1:A:98:MET:CA  | 1:A:98:MET:C  | 1:A:99:GLU:N  | 10       | 1.3           |
| (1,1)   | 1:A:4:TRP:C   | 1:A:5:TYR:N    | 1:A:5:TYR:CA  | 1:A:5:TYR:C   | 5        | 1.3           |
| (1,97)  | 1:A:69:ASN:C  | 1:A:70:LEU:N   | 1:A:70:LEU:CA | 1:A:70:LEU:C  | 4        | 1.2           |
| (1,97)  | 1:A:69:ASN:C  | 1:A:70:LEU:N   | 1:A:70:LEU:CA | 1:A:70:LEU:C  | 7        | 1.2           |
| (1,95)  | 1:A:68:PHE:C  | 1:A:69:ASN:N   | 1:A:69:ASN:CA | 1:A:69:ASN:C  | 16       | 1.2           |
| (1,78)  | 1:A:58:LYS:N  | 1:A:58:LYS:CA  | 1:A:58:LYS:C  | 1:A:59:GLU:N  | 18       | 1.2           |
| (1,68)  | 1:A:49:ASN:N  | 1:A:49:ASN:CA  | 1:A:49:ASN:C  | 1:A:50:SER:N  | 12       | 1.2           |
| (1,67)  | 1:A:48:THR:C  | 1:A:49:ASN:N   | 1:A:49:ASN:CA | 1:A:49:ASN:C  | 12       | 1.2           |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|---------------|----------|---------------|
| (1,56)  | 1:A:43:ILE:N | 1:A:43:ILE:CA | 1:A:43:ILE:C  | 1:A:44:GLU:N  | 15       | 1.2           |
| (1,114) | 1:A:87:THR:N | 1:A:87:THR:CA | 1:A:87:THR:C  | 1:A:88:ALA:N  | 19       | 1.2           |
| (1,112) | 1:A:86:SER:N | 1:A:86:SER:CA | 1:A:86:SER:C  | 1:A:87:THR:N  | 10       | 1.2           |
| (1,92)  | 1:A:67:TYR:N | 1:A:67:TYR:CA | 1:A:67:TYR:C  | 1:A:68:PHE:N  | 12       | 1.1           |
| (1,68)  | 1:A:49:ASN:N | 1:A:49:ASN:CA | 1:A:49:ASN:C  | 1:A:50:SER:N  | 20       | 1.1           |
| (1,21)  | 1:A:17:PHE:C | 1:A:18:VAL:N  | 1:A:18:VAL:CA | 1:A:18:VAL:C  | 6        | 1.1           |
| (1,2)   | 1:A:5:TYR:N  | 1:A:5:TYR:CA  | 1:A:5:TYR:C   | 1:A:6:GLU:N   | 15       | 1.1           |
| (1,138) | 1:A:99:GLU:N | 1:A:99:GLU:CA | 1:A:99:GLU:C  | 1:A:100:ASN:N | 6        | 1.1           |
| (1,136) | 1:A:98:MET:N | 1:A:98:MET:CA | 1:A:98:MET:C  | 1:A:99:GLU:N  | 12       | 1.1           |
| (1,136) | 1:A:98:MET:N | 1:A:98:MET:CA | 1:A:98:MET:C  | 1:A:99:GLU:N  | 17       | 1.1           |
| (1,116) | 1:A:88:ALA:N | 1:A:88:ALA:CA | 1:A:88:ALA:C  | 1:A:89:ALA:N  | 2        | 1.1           |
| (1,104) | 1:A:73:ALA:N | 1:A:73:ALA:CA | 1:A:73:ALA:C  | 1:A:74:ASN:N  | 12       | 1.1           |