



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:16 PM UTC

PDB ID : 2N8Z / pdb\_00002n8z  
BMRB ID : 25871  
Title : Apo form of Calmodulin-Like Domain of Human Non-Muscle alpha-actinin 1  
Authors : Drmota Prebil, S.; Slapsak, U.; de Almeida Ribeiro, E.; Pavsic, M.; Ilc, G.; Zielinska, K.; Hartl, M.; Backman, L.; Plavec, J.; Lenarcic, B.; Djinovic-Carugo, K.  
Deposited on : 2015-10-28

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

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

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

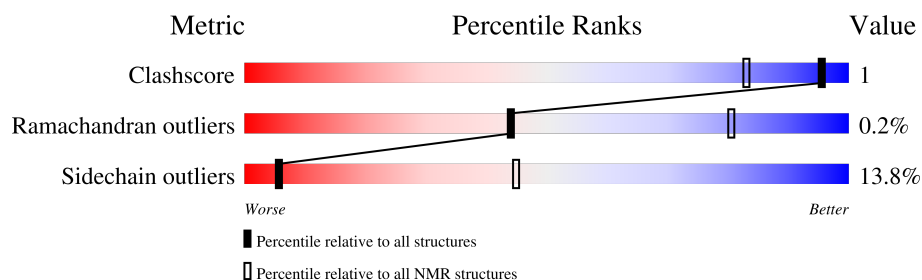
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 84%.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 153    |                  |

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 6 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:746-A:782, A:788-A:815<br>(65) | 0.21              | 6            |
| 2                                    | A:830-A:886 (57)                 | 0.34              | 7            |

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

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

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

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2304 atoms, of which 1114 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-actinin-1.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 153      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2304  | 742 | 1114 | 195 | 244 | 9 |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 740     | GLY      | -      | expression tag | UNP P12814 |
| A     | 741     | SER      | -      | expression tag | UNP P12814 |
| A     | 742     | SER      | -      | expression tag | UNP P12814 |

## 4 Residue-property plots

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

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

- Molecule 1: Alpha-actinin-1

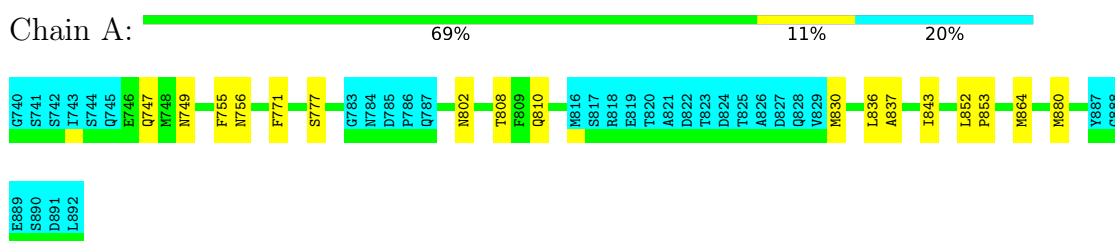


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Alpha-actinin-1



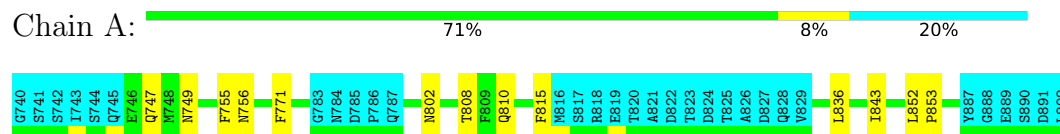
#### 4.2.2 Score per residue for model 2

- Molecule 1: Alpha-actinin-1



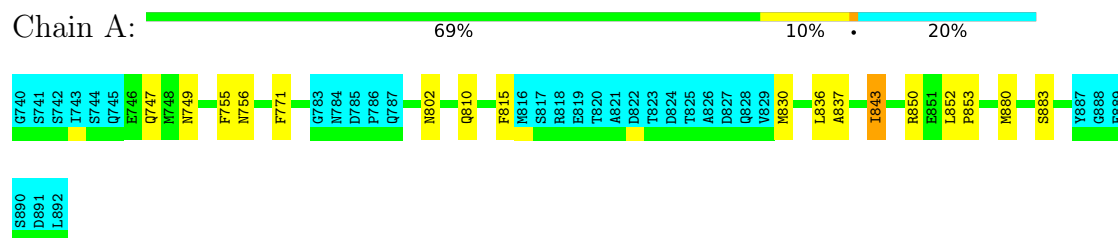
### 4.2.3 Score per residue for model 3

- Molecule 1: Alpha-actinin-1



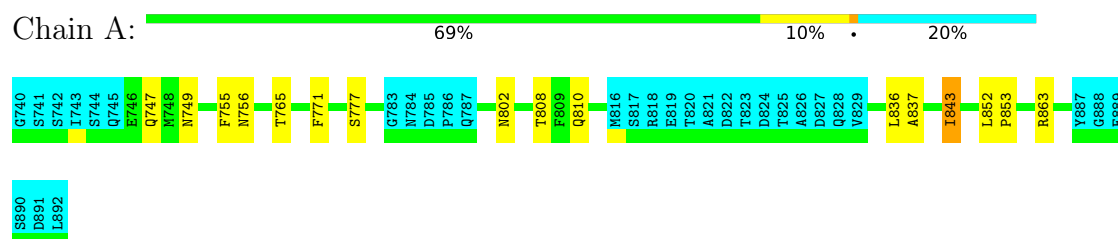
#### 4.2.4 Score per residue for model 4

- Molecule 1: Alpha-actinin-1



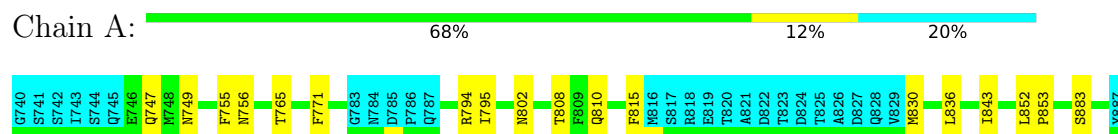
#### 4.2.5 Score per residue for model 5

- Molecule 1: Alpha-actinin-1



#### 4.2.6 Score per residue for model 6 (medoid)

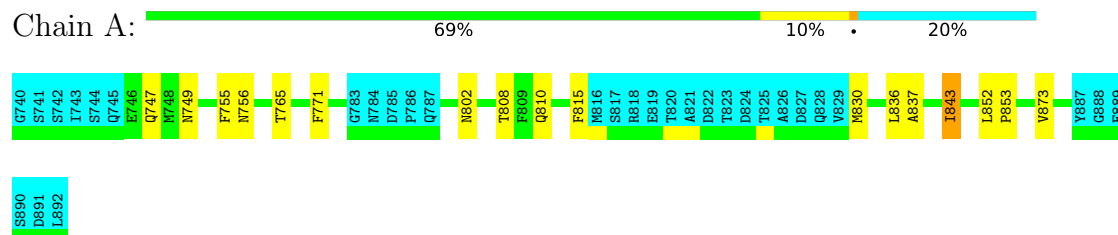
- Molecule 1: Alpha-actinin-1





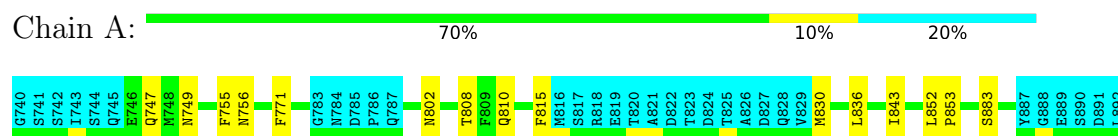
#### 4.2.7 Score per residue for model 7

- Molecule 1: Alpha-actinin-1



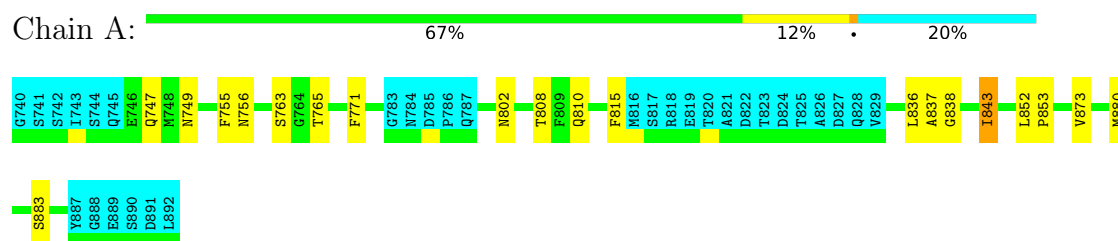
#### 4.2.8 Score per residue for model 8

- Molecule 1: Alpha-actinin-1



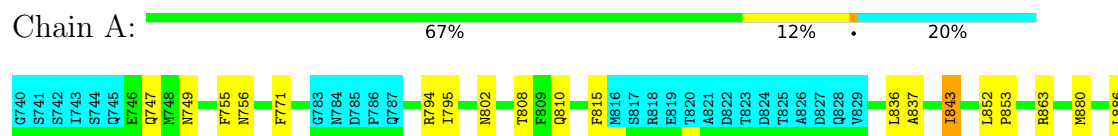
#### 4.2.9 Score per residue for model 9

- Molecule 1: Alpha-actinin-1



#### 4.2.10 Score per residue for model 10

- Molecule 1: Alpha-actinin-1



Y887  
G886  
E889  
S890  
D891  
L892

#### 4.2.11 Score per residue for model 11

- Molecule 1: Alpha-actinin-1

Chain A: 

G740 S741 S742 I743 S744 Q745 E746 Q747 N748 N749 F755 N756 F771 G783 N784 D785 P786 Q787 R794 N802 T808 F809 Q810 F815 M816 S817 R818 E819 T820 A821 D822 D823 T824 D825 A826 D827 Q828 V829 L836 I843 R850 E851 L852 P853 G875 Y887 G888 E889

S890  
D891  
L892

#### 4.2.12 Score per residue for model 12

- Molecule 1: Alpha-actinin-1

Chain A: 

G740 S741 S742 I743 S744 Q745 E746 Q747 N748 N749 F755 N756 D761 F771 G783 N784 D785 P786 Q787 N802 T808 Q810 F815 M816 S817 R818 E819 T820 A821 D822 D823 T824 D825 A826 D827 Q828 V829 M830 L836 I843 T844 M845 L852 P853 P874 Y887 G888 E889 S890

D891  
L892

#### 4.2.13 Score per residue for model 13

- Molecule 1: Alpha-actinin-1

Chain A: 

G740 S741 S742 I743 S744 Q745 E746 Q747 N748 N749 F755 N756 F771 G783 N784 D785 P786 Q787 N802 T808 F809 Q810 F815 M816 S817 R818 E819 T820 A821 D822 D823 T824 D825 A826 D827 Q828 V829 M830 L836 A837 I843 R849 L852 P853 L856 Y887 G888 E889 S890

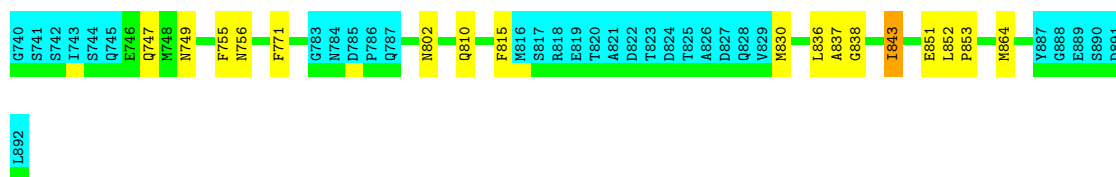
D891  
L892

#### 4.2.14 Score per residue for model 14

- Molecule 1: Alpha-actinin-1

Chain A: 

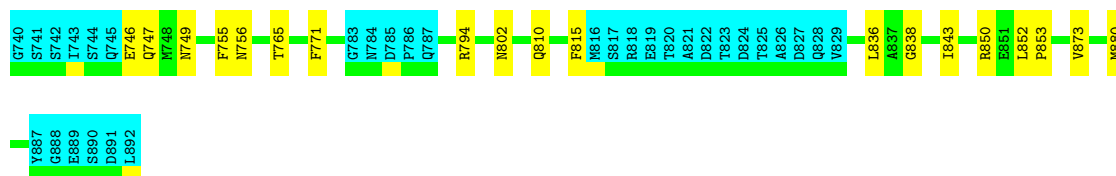




#### 4.2.15 Score per residue for model 15

- Molecule 1: Alpha-actinin-1

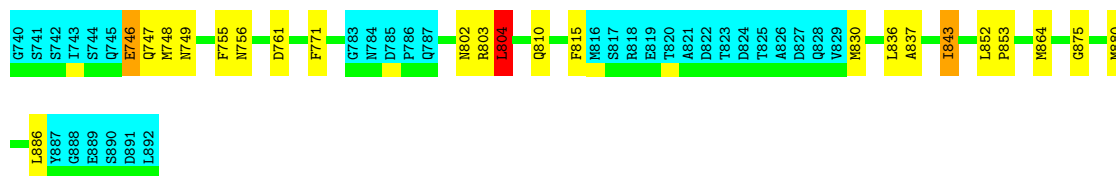
Chain A: 67% 12% 20%



#### 4.2.16 Score per residue for model 16

- Molecule 1: Alpha-actinin-1

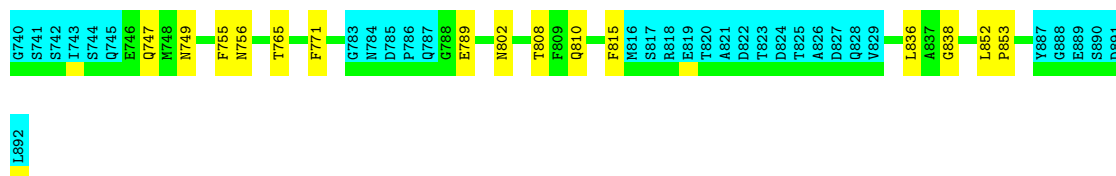
Chain A: 65% 13% 20%



#### 4.2.17 Score per residue for model 17

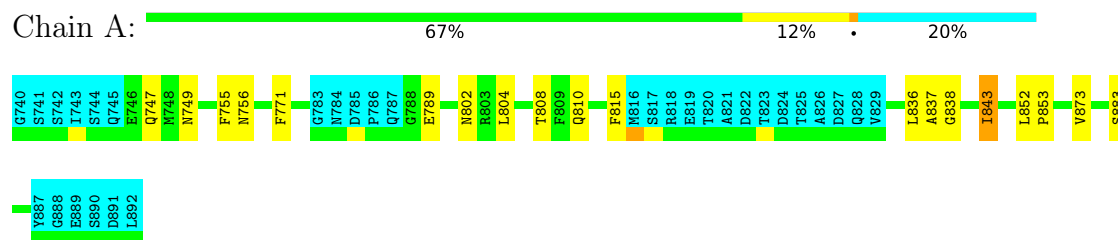
- Molecule 1: Alpha-actinin-1

Chain A: 70% 10% 20%



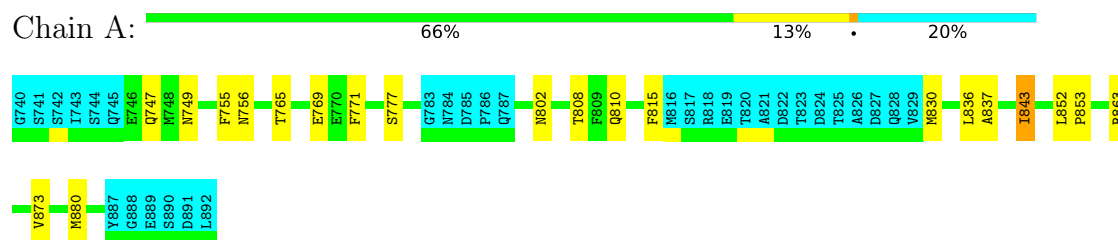
#### 4.2.18 Score per residue for model 18

- Molecule 1: Alpha-actinin-1



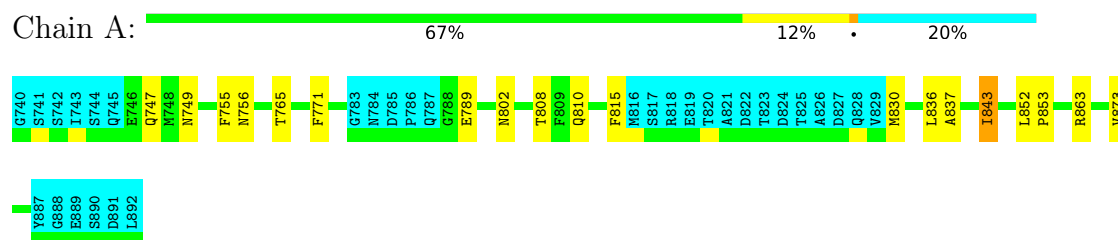
#### 4.2.19 Score per residue for model 19

- Molecule 1: Alpha-actinin-1



#### 4.2.20 Score per residue for model 20

- Molecule 1: Alpha-actinin-1



## 5 Refinement protocol and experimental data overview

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

Of the 20 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 |
|---------------|--------------------|---------|
| CYANA         | structure solution | 3.0     |
| YASARA        | refinement         |         |
| CYANA         | refinement         | 3.0     |

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                       | 1660           |
| Number of shifts mapped to atoms             | 1660           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 84%            |

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                       |
|-----|-------|--------------|----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                  |
| 1   | A     | 0.82±0.04    | 0±0/986 ( 0.0± 0.0%) | 0.93±0.03   | 2±1/1334 ( 0.2± 0.1%) |
| All | All   | 0.82         | 3/19720 ( 0.0%)      | 0.93        | 47/26680 ( 0.2%)      |

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

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 795 | ILE  | N-CA  | 6.19  | 1.53        | 1.46     | 6      | 2     |
| 1   | A     | 837 | ALA  | CA-CB | -5.26 | 1.46        | 1.53     | 2      | 1     |

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

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 853 | PRO  | N-CA-C     | 8.13  | 120.62      | 110.70   | 1      | 20    |
| 1   | A     | 804 | LEU  | CD1-CG-CD2 | 8.13  | 128.68      | 110.80   | 16     | 1     |
| 1   | A     | 873 | VAL  | N-CA-C     | -5.70 | 102.57      | 109.01   | 15     | 7     |
| 1   | A     | 853 | PRO  | CA-C-N     | -5.64 | 112.79      | 119.84   | 13     | 6     |
| 1   | A     | 853 | PRO  | C-N-CA     | -5.64 | 112.79      | 119.84   | 13     | 6     |
| 1   | A     | 761 | ASP  | N-CA-C     | -5.38 | 106.72      | 113.28   | 16     | 2     |
| 1   | A     | 838 | GLY  | N-CA-C     | -5.32 | 107.72      | 114.16   | 14     | 3     |
| 1   | A     | 794 | ARG  | CA-CB-CG   | 5.26  | 124.62      | 114.10   | 11     | 1     |
| 1   | A     | 804 | LEU  | N-CA-C     | -5.12 | 105.88      | 111.82   | 18     | 1     |

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     | 962   | 916      | 916      | 2±1     |
| All | All   | 19240 | 18320    | 18320    | 37      |

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 1.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:802:ASN:HB2  | 1:A:804:LEU:HD11 | 0.71     | 1.61        | 16     | 1     |
| 1:A:837:ALA:HB2  | 1:A:843:ILE:HD12 | 0.68     | 1.63        | 9      | 13    |
| 1:A:804:LEU:HD22 | 1:A:804:LEU:H    | 0.65     | 1.50        | 16     | 1     |
| 1:A:746:GLU:H    | 1:A:746:GLU:CD   | 0.51     | 2.13        | 16     | 2     |
| 1:A:802:ASN:HB2  | 1:A:804:LEU:CD1  | 0.44     | 2.39        | 16     | 1     |
| 1:A:815:PHE:CD1  | 1:A:815:PHE:C    | 0.44     | 2.95        | 11     | 18    |
| 1:A:837:ALA:CB   | 1:A:843:ILE:HD12 | 0.43     | 2.43        | 2      | 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     | 122/153 (80%)   | 116±1 (95±1%) | 5±1 (4±1%) | 0±1 (0±0%) | 44          | 80 |
| All | All   | 2440/3060 (80%) | 2325 (95%)    | 109 (4%)   | 6 (0%)     | 44          | 80 |

All 4 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     | 838 | GLY  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 875 | GLY  | 2              |
| 1   | A     | 874 | PRO  | 1              |
| 1   | A     | 803 | ARG  | 1              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|-------------|----|
| 1   | A     | 102/128 (80%)   | 88±1 (86±1%) | 14±1 (14±1%) | 6           | 45 |
| All | All   | 2040/2560 (80%) | 1759 (86%)   | 281 (14%)    | 6           | 45 |

All 30 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     | 747 | GLN  | 20             |
| 1   | A     | 749 | ASN  | 20             |
| 1   | A     | 755 | PHE  | 20             |
| 1   | A     | 756 | ASN  | 20             |
| 1   | A     | 771 | PHE  | 20             |
| 1   | A     | 810 | GLN  | 20             |
| 1   | A     | 836 | LEU  | 20             |
| 1   | A     | 852 | LEU  | 20             |
| 1   | A     | 802 | ASN  | 19             |
| 1   | A     | 843 | ILE  | 18             |
| 1   | A     | 808 | THR  | 15             |
| 1   | A     | 830 | MET  | 12             |
| 1   | A     | 765 | THR  | 9              |
| 1   | A     | 880 | MET  | 7              |
| 1   | A     | 863 | ARG  | 5              |
| 1   | A     | 883 | SER  | 5              |
| 1   | A     | 886 | LEU  | 4              |
| 1   | A     | 794 | ARG  | 4              |
| 1   | A     | 777 | SER  | 3              |
| 1   | A     | 864 | MET  | 3              |
| 1   | A     | 746 | GLU  | 3              |
| 1   | A     | 850 | ARG  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 789 | GLU  | 3              |
| 1   | A     | 748 | MET  | 2              |
| 1   | A     | 763 | SER  | 1              |
| 1   | A     | 845 | MET  | 1              |
| 1   | A     | 849 | ARG  | 1              |
| 1   | A     | 851 | GLU  | 1              |
| 1   | A     | 804 | LEU  | 1              |
| 1   | A     | 769 | GLU  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 84% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1660 |
| Number of shifts mapped to atoms        | 1660 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 3    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 148      | $-0.16 \pm 0.06$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 138      | $0.16 \pm 0.10$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 141      | $0.20 \pm 0.24$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 1378 atoms were assigned a chemical shift out of a possible 1632. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 476/604 (79%) | 242/245 (99%) | 120/244 (49%)   | 114/115 (99%)   |
| Sidechain | 762/869 (88%) | 521/566 (92%) | 234/272 (86%)   | 7/31 (23%)      |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 140/159 (88%)   | 70/78 (90%)          | 70/79 (89%)           | 0/2 (0%)              |
| Overall  | 1378/1632 (84%) | 833/889 (94%)        | 424/595 (71%)         | 121/148 (82%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1660 atoms were assigned a chemical shift out of a possible 1985. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 588/760 (77%)   | 299/309 (97%)        | 148/306 (48%)         | 141/145 (97%)         |
| Sidechain | 924/1057 (87%)  | 631/685 (92%)        | 282/334 (84%)         | 11/38 (29%)           |
| Aromatic  | 148/168 (88%)   | 74/82 (90%)          | 74/84 (88%)           | 0/2 (0%)              |
| Overall   | 1660/1985 (84%) | 1004/1076 (93%)      | 504/724 (70%)         | 152/185 (82%)         |

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

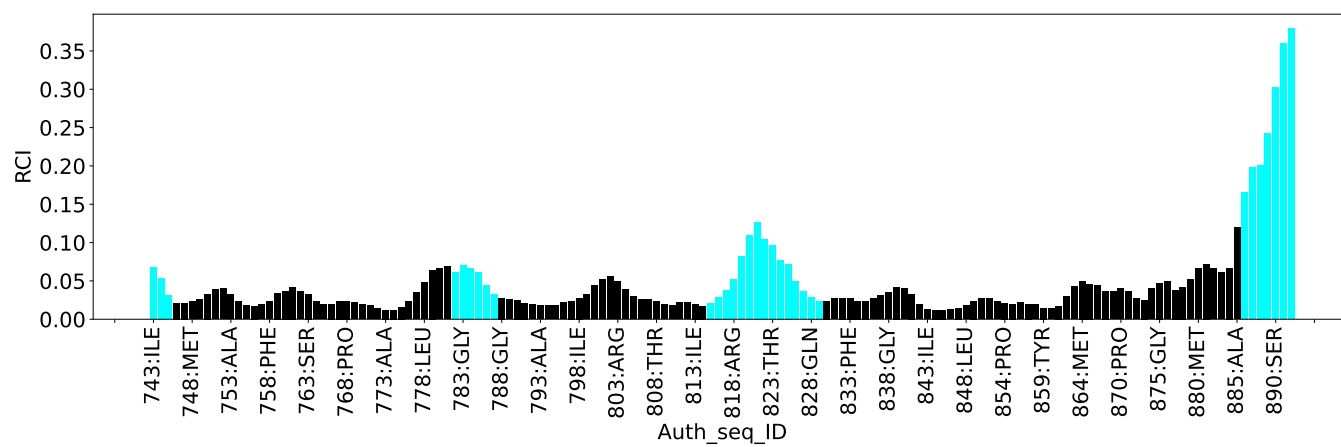
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 778 | LEU  | HD11 | 2.12       | -0.61 – 2.12        | 5.0     |
| 1       | A     | 778 | LEU  | HD12 | 2.12       | -0.61 – 2.12        | 5.0     |
| 1       | A     | 778 | LEU  | HD13 | 2.12       | -0.61 – 2.12        | 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                                | 2723  |
| Intra-residue ( $ i-j =0$ )                              | 636   |
| Sequential ( $ i-j =1$ )                                 | 728   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 768   |
| Long range ( $ i-j \geq 5$ )                             | 591   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 214   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 19.2  |
| Number of long range restraints per residue <sup>1</sup> | 3.9   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 18.1                                   | 0.2     |
| 0.2-0.5 (Medium) | 16.1                                   | 0.5     |
| >0.5 (Large)     | 54.6                                   | 4.22    |

### 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)   | 3.5                                    | 9.97    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

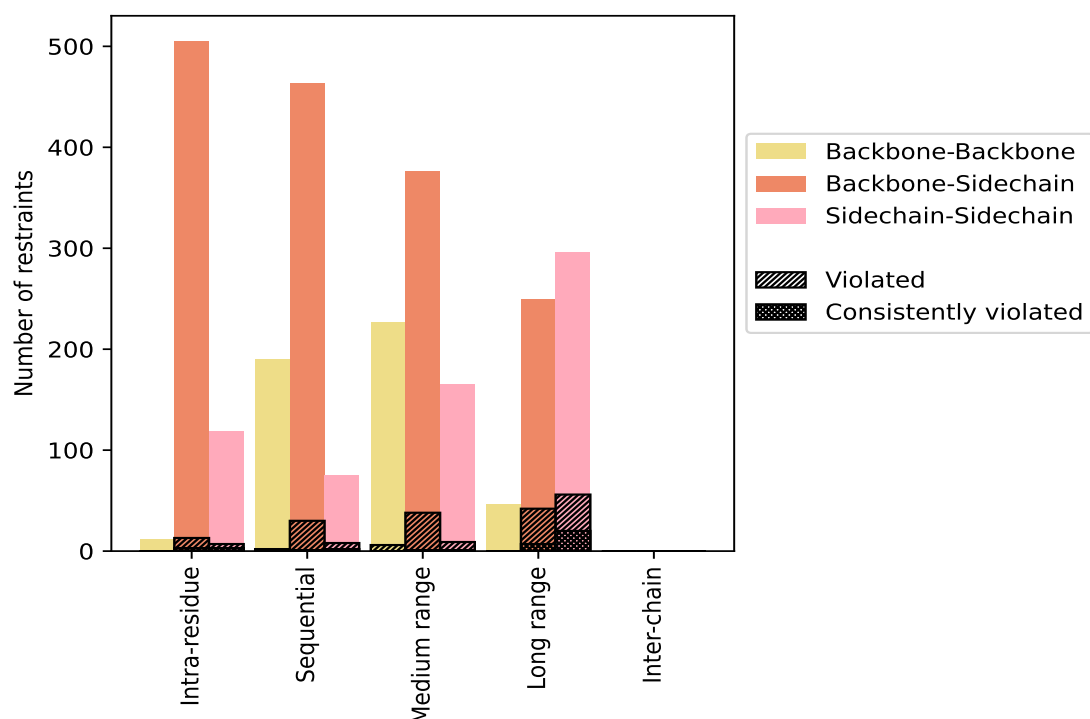
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                     | Consistently Violated <sup>4</sup> |                     |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|----------------------|---------------------|------------------------------------|---------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>      | Count                              | % <sup>2</sup>      | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">636</a>  | <a href="#">23.4</a>  | <a href="#">20</a>    | <a href="#">3.1</a>  | <a href="#">0.7</a> | <a href="#">6</a>                  | <a href="#">0.9</a> | <a href="#">0.2</a> |
| Backbone-Backbone                                          | 12                   | 0.4                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 505                  | 18.5                  | 13                    | 2.6                  | 0.5                 | 3                                  | 0.6                 | 0.1                 |
| Sidechain-Sidechain                                        | 119                  | 4.4                   | 7                     | 5.9                  | 0.3                 | 3                                  | 2.5                 | 0.1                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">728</a>  | <a href="#">26.7</a>  | <a href="#">40</a>    | <a href="#">5.5</a>  | <a href="#">1.5</a> | <a href="#">3</a>                  | <a href="#">0.4</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 190                  | 7.0                   | 2                     | 1.1                  | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 463                  | 17.0                  | 30                    | 6.5                  | 1.1                 | 1                                  | 0.2                 | 0.0                 |
| Sidechain-Sidechain                                        | 75                   | 2.8                   | 8                     | 10.7                 | 0.3                 | 2                                  | 2.7                 | 0.1                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">768</a>  | <a href="#">28.2</a>  | <a href="#">53</a>    | <a href="#">6.9</a>  | <a href="#">1.9</a> | <a href="#">2</a>                  | <a href="#">0.3</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 227                  | 8.3                   | 6                     | 2.6                  | 0.2                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 376                  | 13.8                  | 38                    | 10.1                 | 1.4                 | 1                                  | 0.3                 | 0.0                 |
| Sidechain-Sidechain                                        | 165                  | 6.1                   | 9                     | 5.5                  | 0.3                 | 1                                  | 0.6                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">591</a>  | <a href="#">21.7</a>  | <a href="#">98</a>    | <a href="#">16.6</a> | <a href="#">3.6</a> | <a href="#">27</a>                 | <a href="#">4.6</a> | <a href="#">1.0</a> |
| Backbone-Backbone                                          | 46                   | 1.7                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 249                  | 9.1                   | 42                    | 16.9                 | 1.5                 | 7                                  | 2.8                 | 0.3                 |
| Sidechain-Sidechain                                        | 296                  | 10.9                  | 56                    | 18.9                 | 2.1                 | 20                                 | 6.8                 | 0.7                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| 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                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">2723</a> | <a href="#">100.0</a> | <a href="#">211</a>   | <a href="#">7.7</a>  | <a href="#">7.7</a> | <a href="#">38</a>                 | <a href="#">1.4</a> | <a href="#">1.4</a> |
| Backbone-Backbone                                          | 475                  | 17.4                  | 8                     | 1.7                  | 0.3                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 1593                 | 58.5                  | 123                   | 7.7                  | 4.5                 | 12                                 | 0.8                 | 0.4                 |
| Sidechain-Sidechain                                        | 655                  | 24.1                  | 80                    | 12.2                 | 2.9                 | 26                                 | 4.0                 | 1.0                 |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 9                    | 12              | 9               | 40              | 0               | 70    | 1.05     | 4.19    | 1.1                 | 0.41       |
| 2        | 8                    | 5               | 11              | 56              | 0               | 80    | 1.64     | 4.15    | 1.16                | 1.34       |
| 3        | 13                   | 17              | 14              | 71              | 0               | 115   | 1.35     | 4.19    | 1.22                | 0.94       |
| 4        | 8                    | 9               | 7               | 37              | 0               | 61    | 1.19     | 4.17    | 1.14                | 0.88       |
| 5        | 12                   | 16              | 13              | 69              | 0               | 110   | 1.38     | 4.19    | 1.23                | 0.93       |
| 6        | 8                    | 12              | 14              | 64              | 0               | 98    | 1.38     | 4.22    | 1.2                 | 1.01       |
| 7        | 8                    | 10              | 14              | 66              | 0               | 98    | 1.31     | 4.14    | 1.19                | 0.92       |
| 8        | 8                    | 8               | 10              | 63              | 0               | 89    | 1.49     | 4.13    | 1.18                | 1.23       |
| 9        | 9                    | 13              | 17              | 68              | 0               | 107   | 1.26     | 4.14    | 1.18                | 0.84       |
| 10       | 7                    | 12              | 9               | 41              | 0               | 69    | 1.01     | 4.22    | 1.08                | 0.35       |

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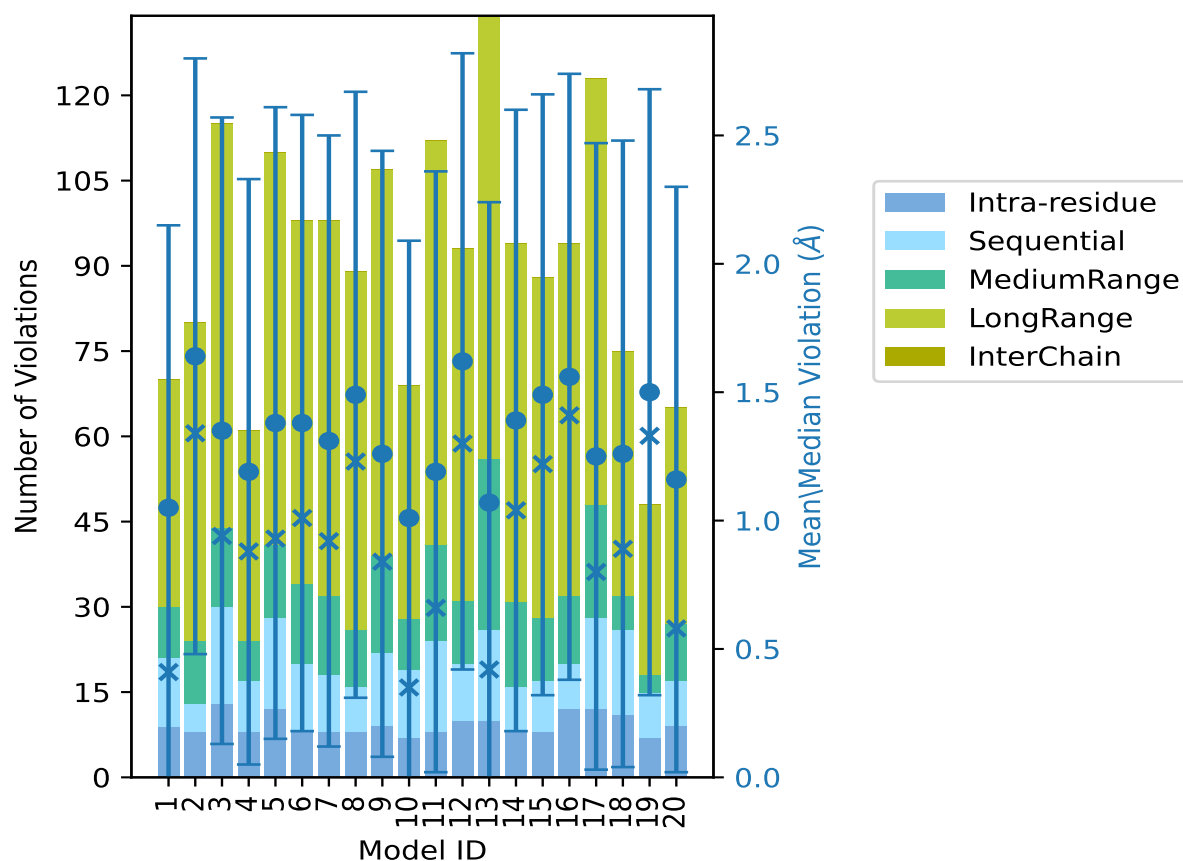
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 8                    | 16              | 17              | 71              | 0               | 112   | 1.19     | 4.16    | 1.17                | 0.66       |
| 12       | 10                   | 10              | 11              | 62              | 0               | 93    | 1.62     | 4.15    | 1.2                 | 1.3        |
| 13       | 10                   | 16              | 30              | 78              | 0               | 134   | 1.07     | 4.13    | 1.17                | 0.42       |
| 14       | 8                    | 8               | 15              | 63              | 0               | 94    | 1.39     | 4.2     | 1.21                | 1.04       |
| 15       | 8                    | 9               | 11              | 60              | 0               | 88    | 1.49     | 4.2     | 1.17                | 1.22       |
| 16       | 12                   | 8               | 12              | 62              | 0               | 94    | 1.56     | 4.16    | 1.18                | 1.41       |
| 17       | 12                   | 16              | 20              | 75              | 0               | 123   | 1.25     | 4.11    | 1.22                | 0.8        |
| 18       | 11                   | 15              | 6               | 43              | 0               | 75    | 1.26     | 4.19    | 1.22                | 0.89       |
| 19       | 7                    | 8               | 3               | 30              | 0               | 48    | 1.5      | 4.17    | 1.18                | 1.33       |
| 20       | 9                    | 8               | 10              | 38              | 0               | 65    | 1.16     | 4.15    | 1.14                | 0.58       |

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

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

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



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

### 9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2512(IR:616, SQ:688, MR:715, LR:493, IC:0) restraints are not violated in the ensemble.

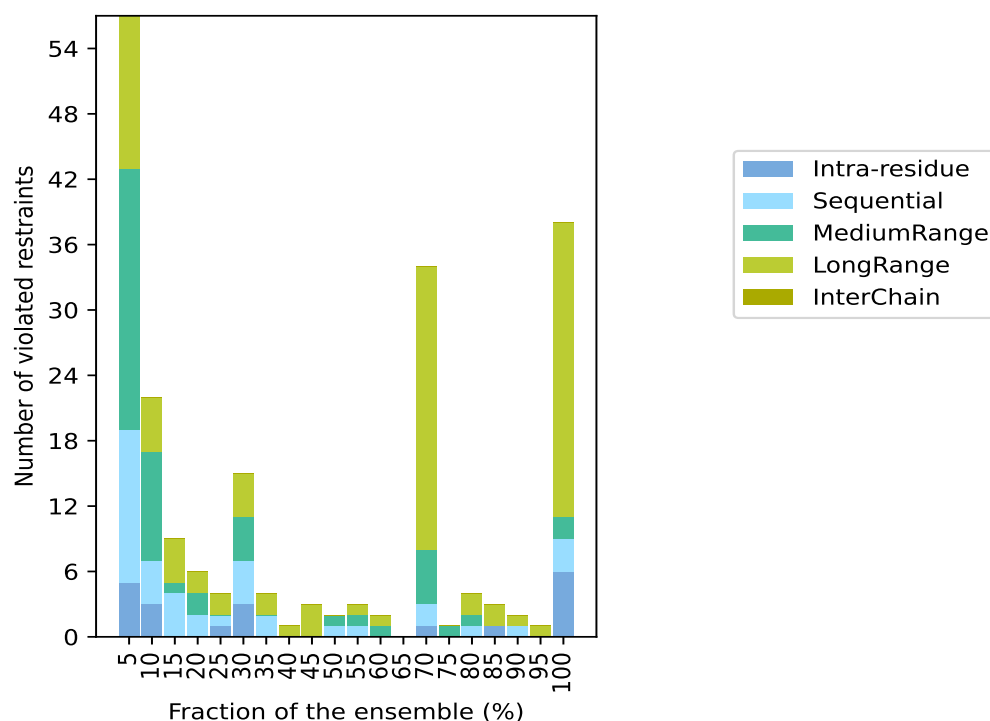
| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 5                             | 14              | 24              | 14              | 0               | 57    | 1                        | 5.0   |
| 3                             | 4               | 10              | 5               | 0               | 22    | 2                        | 10.0  |
| 0                             | 4               | 1               | 4               | 0               | 9     | 3                        | 15.0  |
| 0                             | 2               | 2               | 2               | 0               | 6     | 4                        | 20.0  |
| 1                             | 1               | 0               | 2               | 0               | 4     | 5                        | 25.0  |
| 3                             | 4               | 4               | 4               | 0               | 15    | 6                        | 30.0  |
| 0                             | 2               | 0               | 2               | 0               | 4     | 7                        | 35.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 8                        | 40.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 9                        | 45.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 10                       | 50.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 11                       | 55.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 12                       | 60.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 13                       | 65.0  |
| 1                             | 2               | 5               | 26              | 0               | 34    | 14                       | 70.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 15                       | 75.0  |
| 0                             | 1               | 1               | 2               | 0               | 4     | 16                       | 80.0  |
| 1                             | 0               | 0               | 2               | 0               | 3     | 17                       | 85.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 18                       | 90.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 19                       | 95.0  |
| 6                             | 3               | 2               | 27              | 0               | 38    | 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



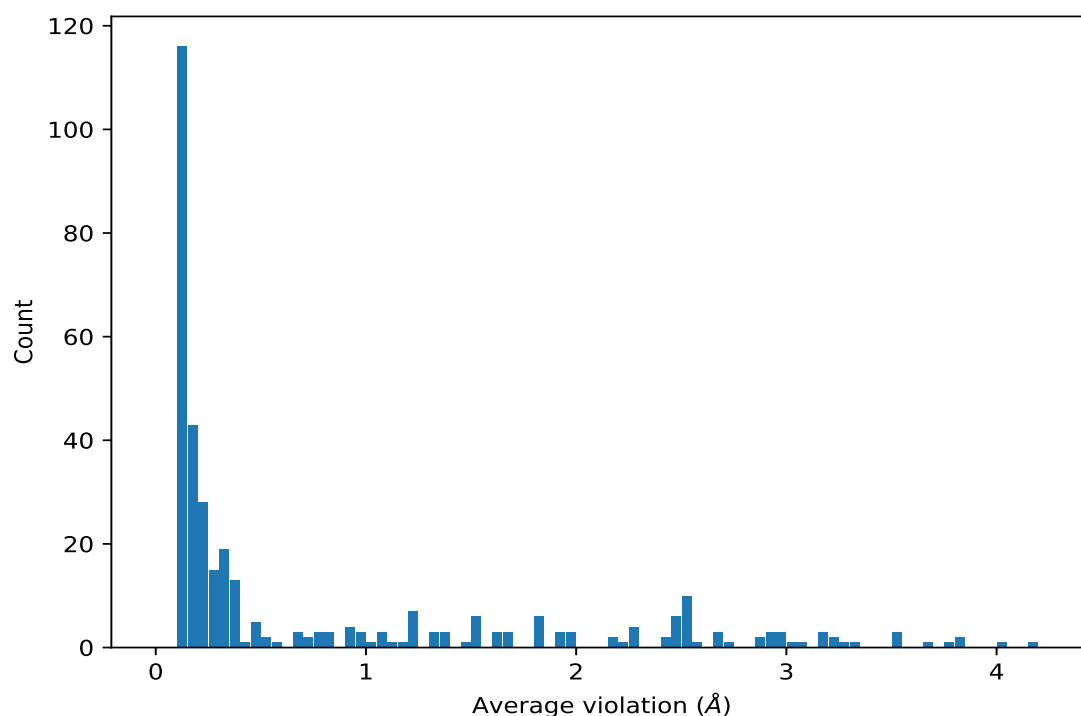
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,931)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HA   | 20                  | 4.17     | 0.03                | 4.16       |
| (1,1898) | 1:771:A:PHE:HD1  | 1:812:A:PHE:H    | 20                  | 3.55     | 0.02                | 3.55       |
| (1,1974) | 1:771:A:PHE:HE1  | 1:813:A:ILE:H    | 20                  | 3.54     | 0.07                | 3.54       |
| (1,936)  | 1:830:A:MET:HB2  | 1:882:A:PHE:HD1  | 20                  | 3.2      | 0.33                | 3.18       |
| (1,400)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG21 | 20                  | 3.17     | 0.04                | 3.17       |
| (1,400)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG22 | 20                  | 3.17     | 0.04                | 3.17       |
| (1,400)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG23 | 20                  | 3.17     | 0.04                | 3.17       |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 20                  | 2.98     | 0.05                | 2.98       |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 20                  | 2.98     | 0.05                | 2.98       |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 20                  | 2.98     | 0.05                | 2.98       |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 20                  | 2.94     | 0.05                | 2.95       |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 20                  | 2.94     | 0.05                | 2.95       |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 20                  | 2.94     | 0.05                | 2.95       |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 20                  | 2.72     | 0.04                | 2.72       |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 20                  | 2.66     | 0.24                | 2.66       |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 20                  | 2.66     | 0.24                | 2.66       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 20                  | 2.66     | 0.24                | 2.66       |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 20                  | 2.5      | 0.2                 | 2.53       |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 20                  | 2.5      | 0.2                 | 2.53       |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 20                  | 2.5      | 0.2                 | 2.53       |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 20                  | 2.5      | 0.2                 | 2.53       |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 20                  | 2.5      | 0.2                 | 2.53       |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 20                  | 2.5      | 0.2                 | 2.53       |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 20                  | 2.48     | 0.31                | 2.49       |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 20                  | 2.48     | 0.31                | 2.49       |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 20                  | 2.48     | 0.31                | 2.49       |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 20                  | 2.42     | 0.12                | 2.44       |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2  | 20                  | 2.28     | 0.03                | 2.28       |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2  | 20                  | 2.28     | 0.03                | 2.28       |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2  | 20                  | 2.28     | 0.03                | 2.28       |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2  | 20                  | 2.26     | 0.06                | 2.26       |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H    | 20                  | 2.15     | 0.07                | 2.16       |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1  | 20                  | 1.96     | 0.05                | 1.96       |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2  | 20                  | 1.96     | 0.05                | 1.96       |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3  | 20                  | 1.96     | 0.05                | 1.96       |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2  | 20                  | 1.94     | 0.06                | 1.95       |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2  | 20                  | 1.94     | 0.06                | 1.95       |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2  | 20                  | 1.94     | 0.06                | 1.95       |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 20                  | 1.81     | 0.25                | 1.8        |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 20                  | 1.81     | 0.25                | 1.8        |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 20                  | 1.81     | 0.25                | 1.8        |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 20                  | 1.81     | 0.25                | 1.8        |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 20                  | 1.81     | 0.25                | 1.8        |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 20                  | 1.81     | 0.25                | 1.8        |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 20                  | 1.69     | 0.29                | 1.59       |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 20                  | 1.69     | 0.29                | 1.59       |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 20                  | 1.69     | 0.29                | 1.59       |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 20                  | 1.62     | 0.26                | 1.71       |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 20                  | 1.62     | 0.26                | 1.71       |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 20                  | 1.62     | 0.26                | 1.71       |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 20                  | 1.54     | 0.05                | 1.54       |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 20                  | 1.54     | 0.05                | 1.54       |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 20                  | 1.54     | 0.05                | 1.54       |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2  | 20                  | 1.5      | 0.45                | 1.34       |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3  | 20                  | 1.5      | 0.45                | 1.34       |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 20                  | 1.46     | 0.04                | 1.47       |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2  | 20                  | 1.36     | 0.06                | 1.34       |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 20                  | 1.32     | 0.3                 | 1.36       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 20                  | 1.32     | 0.3                 | 1.36       |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 20                  | 1.32     | 0.3                 | 1.36       |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 20                  | 1.23     | 0.06                | 1.21       |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 20                  | 1.23     | 0.06                | 1.21       |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 20                  | 1.23     | 0.06                | 1.21       |
| (1,973)  | 1:771:A:PHE:HE1  | 1:812:A:PHE:HD2  | 20                  | 1.16     | 0.07                | 1.18       |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2  | 20                  | 0.99     | 0.03                | 1.0        |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2  | 20                  | 0.99     | 0.03                | 1.0        |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2  | 20                  | 0.99     | 0.03                | 1.0        |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H    | 20                  | 0.95     | 0.1                 | 0.94       |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2  | 20                  | 0.85     | 0.03                | 0.86       |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2  | 20                  | 0.84     | 0.03                | 0.84       |
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 20                  | 0.44     | 0.09                | 0.45       |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 20                  | 0.37     | 0.06                | 0.36       |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 20                  | 0.37     | 0.06                | 0.36       |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 20                  | 0.37     | 0.06                | 0.36       |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 20                  | 0.37     | 0.06                | 0.36       |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 20                  | 0.37     | 0.06                | 0.36       |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 20                  | 0.37     | 0.06                | 0.36       |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD2  | 20                  | 0.37     | 0.06                | 0.36       |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD3  | 20                  | 0.37     | 0.06                | 0.36       |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 20                  | 0.37     | 0.05                | 0.38       |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 20                  | 0.37     | 0.05                | 0.38       |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 20                  | 0.37     | 0.05                | 0.38       |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 20                  | 0.37     | 0.05                | 0.38       |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 20                  | 0.32     | 0.03                | 0.32       |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 20                  | 0.32     | 0.13                | 0.31       |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 20                  | 0.32     | 0.13                | 0.31       |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 20                  | 0.32     | 0.13                | 0.31       |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 20                  | 0.3      | 0.06                | 0.3        |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 19                  | 0.21     | 0.08                | 0.2        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 19                  | 0.21     | 0.08                | 0.2        |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 19                  | 0.21     | 0.08                | 0.2        |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 19                  | 0.21     | 0.08                | 0.2        |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 19                  | 0.21     | 0.08                | 0.2        |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 19                  | 0.21     | 0.08                | 0.2        |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 19                  | 0.21     | 0.08                | 0.2        |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 19                  | 0.21     | 0.08                | 0.2        |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 19                  | 0.21     | 0.08                | 0.2        |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1  | 18                  | 0.67     | 0.21                | 0.7        |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1  | 18                  | 0.67     | 0.21                | 0.7        |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1  | 18                  | 0.67     | 0.21                | 0.7        |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 18                  | 0.18     | 0.05                | 0.17       |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 18                  | 0.18     | 0.05                | 0.17       |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 18                  | 0.18     | 0.05                | 0.17       |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 17                  | 0.25     | 0.06                | 0.25       |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 17                  | 0.18     | 0.03                | 0.18       |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 17                  | 0.18     | 0.03                | 0.18       |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 17                  | 0.18     | 0.03                | 0.18       |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 17                  | 0.16     | 0.04                | 0.16       |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 17                  | 0.16     | 0.04                | 0.16       |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 17                  | 0.16     | 0.04                | 0.16       |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 16                  | 0.23     | 0.09                | 0.2        |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 16                  | 0.23     | 0.09                | 0.2        |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 16                  | 0.23     | 0.09                | 0.2        |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 16                  | 0.23     | 0.08                | 0.25       |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 16                  | 0.23     | 0.08                | 0.25       |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 16                  | 0.23     | 0.08                | 0.25       |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 16                  | 0.23     | 0.08                | 0.25       |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 16                  | 0.23     | 0.08                | 0.25       |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 16                  | 0.23     | 0.08                | 0.25       |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 16                  | 0.15     | 0.03                | 0.16       |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 16                  | 0.15     | 0.03                | 0.16       |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 16                  | 0.15     | 0.03                | 0.16       |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 16                  | 0.15     | 0.03                | 0.16       |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 16                  | 0.15     | 0.03                | 0.16       |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 16                  | 0.15     | 0.03                | 0.16       |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 16                  | 0.15     | 0.04                | 0.15       |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 16                  | 0.15     | 0.04                | 0.15       |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 16                  | 0.15     | 0.04                | 0.15       |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 15                  | 0.23     | 0.06                | 0.23       |
| (1,2381) | 1:867:A:TYR:HD1  | 1:873:A:VAL:H    | 14                  | 4.01     | 0.04                | 4.01       |
| (1,2369) | 1:867:A:TYR:HE1  | 1:872:A:SER:H    | 14                  | 3.84     | 0.13                | 3.8        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,848)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HB2  | 14                  | 3.67     | 0.07                | 3.68       |
| (1,853)  | 1:841:A:ASN:HB2  | 1:867:A:TYR:HE2  | 14                  | 3.52     | 0.14                | 3.52       |
| (1,851)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:H    | 14                  | 3.32     | 0.05                | 3.32       |
| (1,1035) | 1:867:A:TYR:HD1  | 1:872:A:SER:HB2  | 14                  | 3.21     | 0.11                | 3.22       |
| (1,1037) | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB3  | 14                  | 3.02     | 0.05                | 3.03       |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA   | 14                  | 2.9      | 0.05                | 2.88       |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 14                  | 2.88     | 0.04                | 2.86       |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 14                  | 2.57     | 0.06                | 2.6        |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 14                  | 2.55     | 0.06                | 2.53       |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 14                  | 2.55     | 0.06                | 2.53       |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 14                  | 2.55     | 0.06                | 2.53       |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA   | 14                  | 2.54     | 0.25                | 2.46       |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 14                  | 2.47     | 0.05                | 2.46       |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 14                  | 2.47     | 0.05                | 2.46       |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 14                  | 2.47     | 0.05                | 2.46       |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2  | 14                  | 2.41     | 0.16                | 2.42       |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H    | 14                  | 2.17     | 0.04                | 2.17       |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3  | 14                  | 1.51     | 0.12                | 1.5        |
| (1,778)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HB3  | 14                  | 1.24     | 0.09                | 1.23       |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 14                  | 1.22     | 0.05                | 1.22       |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 14                  | 1.22     | 0.05                | 1.22       |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 14                  | 1.22     | 0.05                | 1.22       |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2  | 14                  | 1.1      | 0.21                | 1.08       |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1  | 14                  | 1.07     | 0.03                | 1.08       |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2  | 14                  | 1.07     | 0.03                | 1.08       |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3  | 14                  | 1.07     | 0.03                | 1.08       |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H    | 14                  | 1.02     | 0.75                | 0.64       |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H    | 14                  | 0.95     | 0.2                 | 0.94       |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2  | 14                  | 0.94     | 0.05                | 0.94       |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2  | 14                  | 0.75     | 0.16                | 0.74       |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2  | 14                  | 0.73     | 0.1                 | 0.76       |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2  | 14                  | 0.71     | 0.13                | 0.71       |
| (1,1038) | 1:842:A:TYR:HB2  | 1:867:A:TYR:HD2  | 14                  | 0.54     | 0.11                | 0.54       |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 14                  | 0.52     | 0.12                | 0.54       |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2  | 14                  | 0.49     | 0.23                | 0.42       |
| (1,1034) | 1:867:A:TYR:H    | 1:867:A:TYR:HD1  | 14                  | 0.38     | 0.04                | 0.38       |
| (1,825)  | 1:882:A:PHE:HD1  | 1:883:A:SER:HA   | 14                  | 0.35     | 0.09                | 0.37       |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 14                  | 0.35     | 0.21                | 0.3        |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 14                  | 0.35     | 0.21                | 0.3        |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 14                  | 0.22     | 0.04                | 0.24       |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 14                  | 0.22     | 0.04                | 0.24       |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 14                  | 0.22     | 0.04                | 0.24       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 14                  | 0.19     | 0.07                | 0.18       |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 14                  | 0.19     | 0.07                | 0.18       |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 14                  | 0.19     | 0.07                | 0.18       |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2  | 12                  | 0.45     | 0.26                | 0.32       |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 12                  | 0.18     | 0.06                | 0.16       |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 12                  | 0.18     | 0.06                | 0.16       |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 12                  | 0.18     | 0.06                | 0.16       |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 12                  | 0.18     | 0.06                | 0.16       |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 12                  | 0.18     | 0.06                | 0.16       |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 12                  | 0.18     | 0.06                | 0.16       |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 11                  | 0.13     | 0.02                | 0.12       |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 11                  | 0.13     | 0.02                | 0.12       |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 11                  | 0.13     | 0.02                | 0.12       |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 11                  | 0.13     | 0.03                | 0.12       |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 11                  | 0.13     | 0.03                | 0.12       |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 11                  | 0.13     | 0.03                | 0.12       |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 11                  | 0.12     | 0.01                | 0.11       |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 11                  | 0.12     | 0.01                | 0.11       |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 11                  | 0.12     | 0.01                | 0.11       |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB1  | 10                  | 0.21     | 0.11                | 0.17       |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB2  | 10                  | 0.21     | 0.11                | 0.17       |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB3  | 10                  | 0.21     | 0.11                | 0.17       |
| (1,1486) | 1:775:A:LEU:HD11 | 1:776:A:ILE:H    | 10                  | 0.14     | 0.04                | 0.13       |
| (1,1486) | 1:775:A:LEU:HD12 | 1:776:A:ILE:H    | 10                  | 0.14     | 0.04                | 0.13       |
| (1,1486) | 1:775:A:LEU:HD13 | 1:776:A:ILE:H    | 10                  | 0.14     | 0.04                | 0.13       |
| (1,1031) | 1:842:A:TYR:HD1  | 1:867:A:TYR:HD2  | 9                   | 0.33     | 0.16                | 0.32       |
| (1,1595) | 1:782:A:ILE:HG21 | 1:788:A:GLY:H    | 9                   | 0.14     | 0.04                | 0.13       |
| (1,1595) | 1:782:A:ILE:HG22 | 1:788:A:GLY:H    | 9                   | 0.14     | 0.04                | 0.13       |
| (1,1595) | 1:782:A:ILE:HG23 | 1:788:A:GLY:H    | 9                   | 0.14     | 0.04                | 0.13       |
| (1,116)  | 1:765:A:THR:HG21 | 1:771:A:PHE:HZ   | 9                   | 0.14     | 0.03                | 0.13       |
| (1,116)  | 1:765:A:THR:HG22 | 1:771:A:PHE:HZ   | 9                   | 0.14     | 0.03                | 0.13       |
| (1,116)  | 1:765:A:THR:HG23 | 1:771:A:PHE:HZ   | 9                   | 0.14     | 0.03                | 0.13       |
| (1,764)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HB2  | 8                   | 0.13     | 0.02                | 0.13       |
| (1,764)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HB2  | 8                   | 0.13     | 0.02                | 0.13       |
| (1,764)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HB2  | 8                   | 0.13     | 0.02                | 0.13       |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD11 | 7                   | 0.16     | 0.03                | 0.15       |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD12 | 7                   | 0.16     | 0.03                | 0.15       |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD13 | 7                   | 0.16     | 0.03                | 0.15       |
| (1,1543) | 1:776:A:ILE:HD11 | 1:782:A:ILE:H    | 7                   | 0.13     | 0.03                | 0.13       |
| (1,1543) | 1:776:A:ILE:HD12 | 1:782:A:ILE:H    | 7                   | 0.13     | 0.03                | 0.13       |
| (1,1543) | 1:776:A:ILE:HD13 | 1:782:A:ILE:H    | 7                   | 0.13     | 0.03                | 0.13       |
| (1,1120) | 1:743:A:ILE:HD11 | 1:744:A:SER:H    | 7                   | 0.13     | 0.02                | 0.12       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1120) | 1:743:A:ILE:HD12 | 1:744:A:SER:H    | 7                   | 0.13     | 0.02                | 0.12       |
| (1,1120) | 1:743:A:ILE:HD13 | 1:744:A:SER:H    | 7                   | 0.13     | 0.02                | 0.12       |
| (1,1490) | 1:776:A:ILE:HG21 | 1:777:A:SER:H    | 7                   | 0.11     | 0.01                | 0.12       |
| (1,1490) | 1:776:A:ILE:HG22 | 1:777:A:SER:H    | 7                   | 0.11     | 0.01                | 0.12       |
| (1,1490) | 1:776:A:ILE:HG23 | 1:777:A:SER:H    | 7                   | 0.11     | 0.01                | 0.12       |
| (1,2348) | 1:865:A:ALA:H    | 1:887:A:TYR:HE1  | 6                   | 3.82     | 0.35                | 3.99       |
| (1,1075) | 1:865:A:ALA:HA   | 1:887:A:TYR:HE1  | 6                   | 3.79     | 0.28                | 3.84       |
| (1,1073) | 1:865:A:ALA:HA   | 1:887:A:TYR:HD1  | 6                   | 3.28     | 0.2                 | 3.17       |
| (1,1074) | 1:866:A:PRO:HD3  | 1:887:A:TYR:HE1  | 6                   | 3.06     | 0.35                | 3.04       |
| (1,1072) | 1:886:A:LEU:HA   | 1:887:A:TYR:HD1  | 6                   | 2.22     | 0.19                | 2.3        |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA2  | 6                   | 1.4      | 0.3                 | 1.31       |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA3  | 6                   | 1.4      | 0.3                 | 1.31       |
| (1,1071) | 1:887:A:TYR:HB3  | 1:887:A:TYR:HD1  | 6                   | 0.92     | 0.01                | 0.92       |
| (1,1644) | 1:792:A:PHE:H    | 1:794:A:ARG:HG2  | 6                   | 0.8      | 0.48                | 0.9        |
| (1,2493) | 1:887:A:TYR:H    | 1:887:A:TYR:HD1  | 6                   | 0.79     | 0.2                 | 0.86       |
| (1,2494) | 1:887:A:TYR:H    | 1:887:A:TYR:HE1  | 6                   | 0.79     | 0.24                | 0.86       |
| (1,2716) | 1:887:A:TYR:HE2  | 1:888:A:GLY:HA2  | 6                   | 0.49     | 0.45                | 0.32       |
| (1,2716) | 1:887:A:TYR:HE2  | 1:888:A:GLY:HA3  | 6                   | 0.49     | 0.45                | 0.32       |
| (1,1856) | 1:808:A:THR:HG21 | 1:810:A:GLN:H    | 6                   | 0.16     | 0.03                | 0.16       |
| (1,1856) | 1:808:A:THR:HG22 | 1:810:A:GLN:H    | 6                   | 0.16     | 0.03                | 0.16       |
| (1,1856) | 1:808:A:THR:HG23 | 1:810:A:GLN:H    | 6                   | 0.16     | 0.03                | 0.16       |
| (1,1149) | 1:743:A:ILE:HG21 | 1:747:A:GLN:HE22 | 6                   | 0.14     | 0.04                | 0.13       |
| (1,1149) | 1:743:A:ILE:HG22 | 1:747:A:GLN:HE22 | 6                   | 0.14     | 0.04                | 0.13       |
| (1,1149) | 1:743:A:ILE:HG23 | 1:747:A:GLN:HE22 | 6                   | 0.14     | 0.04                | 0.13       |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB1  | 6                   | 0.13     | 0.02                | 0.13       |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB2  | 6                   | 0.13     | 0.02                | 0.13       |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB3  | 6                   | 0.13     | 0.02                | 0.13       |
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD21 | 6                   | 0.12     | 0.03                | 0.12       |
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD22 | 6                   | 0.12     | 0.03                | 0.12       |
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD23 | 6                   | 0.12     | 0.03                | 0.12       |
| (1,1167) | 1:743:A:ILE:HG13 | 1:748:A:MET:H    | 5                   | 0.21     | 0.08                | 0.2        |
| (1,1971) | 1:820:A:THR:HG21 | 1:821:A:ALA:H    | 5                   | 0.19     | 0.04                | 0.17       |
| (1,1971) | 1:820:A:THR:HG22 | 1:821:A:ALA:H    | 5                   | 0.19     | 0.04                | 0.17       |
| (1,1971) | 1:820:A:THR:HG23 | 1:821:A:ALA:H    | 5                   | 0.19     | 0.04                | 0.17       |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD2  | 5                   | 0.15     | 0.01                | 0.14       |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD3  | 5                   | 0.15     | 0.01                | 0.14       |
| (1,1798) | 1:800:A:ASP:HB3  | 1:806:A:VAL:H    | 5                   | 0.12     | 0.02                | 0.11       |
| (1,1632) | 1:791:A:GLU:H    | 1:794:A:ARG:HG2  | 4                   | 0.57     | 0.26                | 0.71       |
| (1,1168) | 1:772:A:LYS:HD3  | 1:784:A:ASN:H    | 4                   | 0.47     | 0.16                | 0.5        |
| (1,1671) | 1:794:A:ARG:HG2  | 1:795:A:ILE:H    | 4                   | 0.24     | 0.09                | 0.24       |
| (1,1118) | 1:743:A:ILE:HG13 | 1:744:A:SER:H    | 4                   | 0.16     | 0.02                | 0.16       |
| (1,2038) | 1:836:A:LEU:HD11 | 1:848:A:LEU:H    | 4                   | 0.14     | 0.04                | 0.13       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2038) | 1:836:A:LEU:HD12 | 1:848:A:LEU:H    | 4                   | 0.14     | 0.04                | 0.13       |
| (1,2038) | 1:836:A:LEU:HD13 | 1:848:A:LEU:H    | 4                   | 0.14     | 0.04                | 0.13       |
| (1,251)  | 1:773:A:ALA:HA   | 1:776:A:ILE:HG21 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,251)  | 1:773:A:ALA:HA   | 1:776:A:ILE:HG22 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,251)  | 1:773:A:ALA:HA   | 1:776:A:ILE:HG23 | 4                   | 0.12     | 0.01                | 0.12       |
| (1,561)  | 1:830:A:MET:HE1  | 1:879:A:TYR:HA   | 3                   | 0.17     | 0.03                | 0.16       |
| (1,561)  | 1:830:A:MET:HE2  | 1:879:A:TYR:HA   | 3                   | 0.17     | 0.03                | 0.16       |
| (1,561)  | 1:830:A:MET:HE3  | 1:879:A:TYR:HA   | 3                   | 0.17     | 0.03                | 0.16       |
| (1,2585) | 1:793:A:ALA:HB1  | 1:794:A:ARG:HD2  | 3                   | 0.16     | 0.05                | 0.14       |
| (1,2585) | 1:793:A:ALA:HB1  | 1:794:A:ARG:HD3  | 3                   | 0.16     | 0.05                | 0.14       |
| (1,2585) | 1:793:A:ALA:HB2  | 1:794:A:ARG:HD2  | 3                   | 0.16     | 0.05                | 0.14       |
| (1,2585) | 1:793:A:ALA:HB2  | 1:794:A:ARG:HD3  | 3                   | 0.16     | 0.05                | 0.14       |
| (1,2585) | 1:793:A:ALA:HB3  | 1:794:A:ARG:HD2  | 3                   | 0.16     | 0.05                | 0.14       |
| (1,2585) | 1:793:A:ALA:HB3  | 1:794:A:ARG:HD3  | 3                   | 0.16     | 0.05                | 0.14       |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG11 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG12 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG13 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG21 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG22 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG23 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG11 | 3                   | 0.13     | 0.01                | 0.12       |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG12 | 3                   | 0.13     | 0.01                | 0.12       |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG13 | 3                   | 0.13     | 0.01                | 0.12       |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG21 | 3                   | 0.13     | 0.01                | 0.12       |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG22 | 3                   | 0.13     | 0.01                | 0.12       |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG23 | 3                   | 0.13     | 0.01                | 0.12       |
| (1,134)  | 1:766:A:LEU:HG   | 1:771:A:PHE:H    | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1892) | 1:765:A:THR:HG21 | 1:811:A:ALA:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1892) | 1:765:A:THR:HG22 | 1:811:A:ALA:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1892) | 1:765:A:THR:HG23 | 1:811:A:ALA:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG21 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG22 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG23 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1674) | 1:795:A:ILE:H    | 1:796:A:MET:HG2  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1893) | 1:799:A:VAL:HG11 | 1:811:A:ALA:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1893) | 1:799:A:VAL:HG12 | 1:811:A:ALA:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1893) | 1:799:A:VAL:HG13 | 1:811:A:ALA:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG11 | 2                   | 0.29     | 0.13                | 0.29       |
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG12 | 2                   | 0.29     | 0.13                | 0.29       |
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG13 | 2                   | 0.29     | 0.13                | 0.29       |
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG21 | 2                   | 0.29     | 0.13                | 0.29       |
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG22 | 2                   | 0.29     | 0.13                | 0.29       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG23 | 2                   | 0.29     | 0.13                | 0.29       |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG11 | 2                   | 0.28     | 0.18                | 0.28       |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG12 | 2                   | 0.28     | 0.18                | 0.28       |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG13 | 2                   | 0.28     | 0.18                | 0.28       |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG21 | 2                   | 0.28     | 0.18                | 0.28       |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG22 | 2                   | 0.28     | 0.18                | 0.28       |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG23 | 2                   | 0.28     | 0.18                | 0.28       |
| (1,2072) | 1:838:A:GLY:H    | 1:839:A:ASP:HA   | 2                   | 0.26     | 0.1                 | 0.26       |
| (1,1122) | 1:745:A:GLN:HB2  | 1:745:A:GLN:HE22 | 2                   | 0.24     | 0.07                | 0.24       |
| (1,1554) | 1:772:A:LYS:HD2  | 1:783:A:GLY:H    | 2                   | 0.19     | 0.06                | 0.19       |
| (1,2587) | 1:794:A:ARG:HD2  | 1:795:A:ILE:H    | 2                   | 0.18     | 0.02                | 0.18       |
| (1,2587) | 1:794:A:ARG:HD3  | 1:795:A:ILE:H    | 2                   | 0.18     | 0.02                | 0.18       |
| (1,571)  | 1:832:A:SER:HB2  | 1:835:A:ILE:HD11 | 2                   | 0.16     | 0.03                | 0.16       |
| (1,571)  | 1:832:A:SER:HB2  | 1:835:A:ILE:HD12 | 2                   | 0.16     | 0.03                | 0.16       |
| (1,571)  | 1:832:A:SER:HB2  | 1:835:A:ILE:HD13 | 2                   | 0.16     | 0.03                | 0.16       |
| (1,1068) | 1:838:A:GLY:HA2  | 1:879:A:TYR:HE1  | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,2591) | 1:803:A:ARG:H    | 1:803:A:ARG:HG2  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2591) | 1:803:A:ARG:H    | 1:803:A:ARG:HG3  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,43)   | 1:743:A:ILE:HD11 | 1:748:A:MET:HE1  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,43)   | 1:743:A:ILE:HD11 | 1:748:A:MET:HE2  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,43)   | 1:743:A:ILE:HD11 | 1:748:A:MET:HE3  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,43)   | 1:743:A:ILE:HD12 | 1:748:A:MET:HE1  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,43)   | 1:743:A:ILE:HD12 | 1:748:A:MET:HE2  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,43)   | 1:743:A:ILE:HD12 | 1:748:A:MET:HE3  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,43)   | 1:743:A:ILE:HD13 | 1:748:A:MET:HE1  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,43)   | 1:743:A:ILE:HD13 | 1:748:A:MET:HE2  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,43)   | 1:743:A:ILE:HD13 | 1:748:A:MET:HE3  | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,307)  | 1:785:A:ASP:HB3  | 1:787:A:GLN:H    | 2                   | 0.14     | 0.03                | 0.14       |
| (1,1492) | 1:798:A:ILE:HA   | 1:800:A:ASP:H    | 2                   | 0.13     | 0.01                | 0.13       |
| (1,1527) | 1:775:A:LEU:HD11 | 1:780:A:TYR:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1527) | 1:775:A:LEU:HD12 | 1:780:A:TYR:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1527) | 1:775:A:LEU:HD13 | 1:780:A:TYR:H    | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2720) | 1:890:A:SER:HB2  | 1:892:A:LEU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2720) | 1:890:A:SER:HB3  | 1:892:A:LEU:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,12)   | 1:798:A:ILE:HG21 | 1:800:A:ASP:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,12)   | 1:798:A:ILE:HG22 | 1:800:A:ASP:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,12)   | 1:798:A:ILE:HG23 | 1:800:A:ASP:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2621) | 1:824:A:ASP:HB2  | 1:826:A:ALA:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2621) | 1:824:A:ASP:HB3  | 1:826:A:ALA:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1601) | 1:789:A:GLU:H    | 1:789:A:GLU:HG3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2008) | 1:827:A:ASP:HB2  | 1:828:A:GLN:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2063) | 1:835:A:ILE:H    | 1:837:A:ALA:H    | 2                   | 0.11     | 0.01                | 0.11       |

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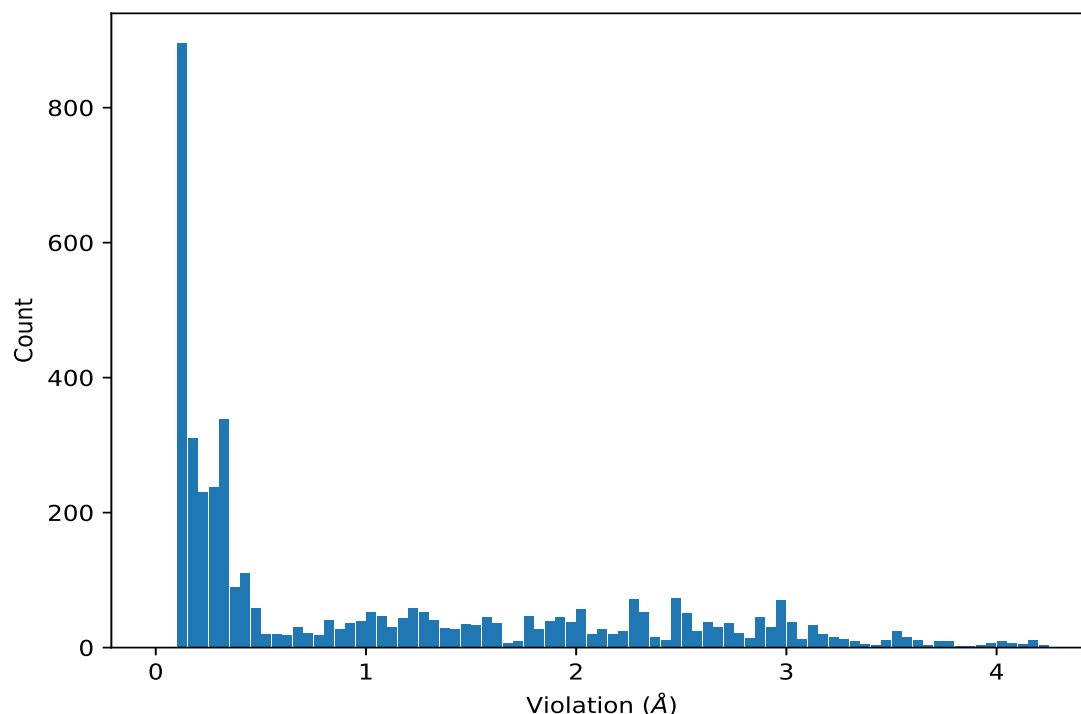
| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1742) | 1:802:A:ASN:H    | 1:804:A:LEU:HD21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1742) | 1:802:A:ASN:H    | 1:804:A:LEU:HD22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1742) | 1:802:A:ASN:H    | 1:804:A:LEU:HD23 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,727)  | 1:782:A:ILE:HD11 | 1:791:A:GLU:HB2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,727)  | 1:782:A:ILE:HD12 | 1:791:A:GLU:HB2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,727)  | 1:782:A:ILE:HD13 | 1:791:A:GLU:HB2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1526) | 1:776:A:ILE:HG21 | 1:780:A:TYR:H    | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1526) | 1:776:A:ILE:HG22 | 1:780:A:TYR:H    | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,1526) | 1:776:A:ILE:HG23 | 1:780:A:TYR:H    | 2                   | 0.1      | 0.0                 | 0.1        |

<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) |
|----------|-----------------|-----------------|----------|---------------|
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 6        | 4.22          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 10       | 4.22          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 14       | 4.2           |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 15       | 4.2           |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 1        | 4.19          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 3        | 4.19          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 5        | 4.19          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 18       | 4.19          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 4        | 4.17          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 19       | 4.17          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 11       | 4.16          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 16       | 4.16          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 2        | 4.15          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 12       | 4.15          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 20       | 4.15          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 7        | 4.14          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 9        | 4.14          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 8        | 4.13          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 13       | 4.13          |
| (1,931)  | 1:771:A:PHE:HD1 | 1:812:A:PHE:HA  | 17       | 4.11          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 9        | 4.07          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 13       | 4.07          |
| (1,2348) | 1:865:A:ALA:H   | 1:887:A:TYR:HE1 | 18       | 4.07          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 13       | 4.06          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 17       | 4.05          |
| (1,2348) | 1:865:A:ALA:H   | 1:887:A:TYR:HE1 | 3        | 4.05          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 6        | 4.04          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 8        | 4.03          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 16       | 4.03          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 17       | 4.03          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 12       | 4.02          |
| (1,1075) | 1:865:A:ALA:HA  | 1:887:A:TYR:HE1 | 18       | 4.02          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 11       | 4.01          |
| (1,1075) | 1:865:A:ALA:HA  | 1:887:A:TYR:HE1 | 3        | 4.01          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 11       | 4.0           |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 2        | 3.99          |
| (1,2348) | 1:865:A:ALA:H   | 1:887:A:TYR:HE1 | 5        | 3.99          |
| (1,2348) | 1:865:A:ALA:H   | 1:887:A:TYR:HE1 | 12       | 3.99          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 5        | 3.98          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 7        | 3.98          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 14       | 3.98          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 15       | 3.98          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 14       | 3.94          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 3        | 3.92          |
| (1,2381) | 1:867:A:TYR:HD1 | 1:873:A:VAL:H   | 3        | 3.91          |
| (1,1075) | 1:865:A:ALA:HA  | 1:887:A:TYR:HE1 | 12       | 3.86          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 8        | 3.85          |
| (1,1075) | 1:865:A:ALA:HA  | 1:887:A:TYR:HE1 | 5        | 3.83          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 9        | 3.81          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 2        | 3.8           |
| (1,1075) | 1:865:A:ALA:HA  | 1:887:A:TYR:HE1 | 17       | 3.8           |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 9        | 3.79          |
| (1,2348) | 1:865:A:ALA:H   | 1:887:A:TYR:HE1 | 17       | 3.78          |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 6        | 3.78          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2 | 9        | 3.77          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2 | 13       | 3.77          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 7        | 3.75          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 15       | 3.75          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 12       | 3.74          |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 2        | 3.73          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1 | 11       | 3.72          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1 | 16       | 3.72          |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 13       | 3.72          |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 15       | 3.72          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 5        | 3.71          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 16       | 3.71          |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 8        | 3.7           |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 14       | 3.68          |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 16       | 3.67          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2 | 2        | 3.66          |
| (1,2369) | 1:867:A:TYR:HE1 | 1:872:A:SER:H   | 6        | 3.65          |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 5        | 3.65          |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 12       | 3.64          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 15       | 3.63          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1 | 12       | 3.63          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 10       | 3.62          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 16       | 3.62          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 6        | 3.61          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2 | 17       | 3.61          |
| (1,1073) | 1:865:A:ALA:HA  | 1:887:A:TYR:HD1 | 18       | 3.6           |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 3        | 3.6           |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 12       | 3.59          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 19       | 3.59          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 10       | 3.59          |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 11       | 3.59          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 6        | 3.58          |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 7        | 3.58          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 14       | 3.57          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 15       | 3.57          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 16       | 3.57          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 18       | 3.57          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 19       | 3.57          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 5        | 3.56          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 14       | 3.56          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 20       | 3.56          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2 | 3        | 3.56          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 8        | 3.55          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 11       | 3.55          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 1        | 3.55          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 4        | 3.55          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 5        | 3.55          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 7        | 3.55          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 12       | 3.55          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 17       | 3.55          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 3        | 3.54          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 7        | 3.54          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 9        | 3.54          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2 | 6        | 3.54          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2 | 14       | 3.54          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 8        | 3.53          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 9        | 3.53          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 11       | 3.53          |
| (1,848)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB2 | 17       | 3.53          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 1        | 3.52          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 20       | 3.52          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 2        | 3.52          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 3        | 3.52          |
| (1,1898) | 1:771:A:PHE:HD1 | 1:812:A:PHE:H   | 13       | 3.52          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 4        | 3.51          |
| (1,1073) | 1:865:A:ALA:HA  | 1:887:A:TYR:HD1 | 3        | 3.5           |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H   | 17       | 3.49          |
| (1,1074) | 1:866:A:PRO:HD3 | 1:887:A:TYR:HE1 | 3        | 3.49          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1 | 6        | 3.49          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1 | 13       | 3.49          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2 | 12       | 3.49          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H    | 2        | 3.48          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H    | 18       | 3.48          |
| (1,1074) | 1:866:A:PRO:HD3 | 1:887:A:TYR:HE1  | 18       | 3.48          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1  | 20       | 3.48          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2  | 15       | 3.48          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2  | 8        | 3.46          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 13       | 3.44          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2  | 16       | 3.42          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 9        | 3.41          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1  | 19       | 3.41          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2  | 7        | 3.38          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 17       | 3.38          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 6        | 3.36          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 8        | 3.36          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 7        | 3.35          |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2  | 5        | 3.33          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 15       | 3.33          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 16       | 3.33          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1  | 17       | 3.32          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 2        | 3.32          |
| (1,1974) | 1:771:A:PHE:HE1 | 1:813:A:ILE:H    | 13       | 3.31          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 2        | 3.31          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 6        | 3.31          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 12       | 3.31          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 11       | 3.3           |
| (1,853)  | 1:841:A:ASN:HB2 | 1:867:A:TYR:HE2  | 11       | 3.29          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 5        | 3.29          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 9        | 3.29          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 15       | 3.28          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1  | 5        | 3.28          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 13       | 3.27          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 3        | 3.27          |
| (1,851)  | 1:867:A:TYR:HE1 | 1:873:A:VAL:H    | 14       | 3.26          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 8        | 3.25          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 17       | 3.25          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 17       | 3.25          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 17       | 3.25          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1  | 8        | 3.24          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 14       | 3.23          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 18       | 3.22          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 18       | 3.22          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 18       | 3.22          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 16       | 3.21          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 7        | 3.21          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 7        | 3.21          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 7        | 3.21          |
| (1,1075) | 1:865:A:ALA:HA  | 1:887:A:TYR:HE1  | 16       | 3.2           |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 11       | 3.2           |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 11       | 3.2           |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 11       | 3.2           |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 12       | 3.2           |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 12       | 3.2           |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 12       | 3.2           |
| (1,1073) | 1:865:A:ALA:HA  | 1:887:A:TYR:HD1  | 12       | 3.19          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 1        | 3.19          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 1        | 3.19          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 1        | 3.19          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 2        | 3.19          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 2        | 3.19          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 2        | 3.19          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 19       | 3.19          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 19       | 3.19          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 19       | 3.19          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 8        | 3.18          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 8        | 3.18          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 8        | 3.18          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 20       | 3.18          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 20       | 3.18          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 20       | 3.18          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 5        | 3.17          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 13       | 3.16          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 13       | 3.16          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 13       | 3.16          |
| (1,1073) | 1:865:A:ALA:HA  | 1:887:A:TYR:HD1  | 5        | 3.15          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 12       | 3.15          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 4        | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 4        | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 4        | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 5        | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 5        | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 5        | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 6        | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 6        | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 6        | 3.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 9        | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 9        | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 9        | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 10       | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 10       | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 10       | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 14       | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 14       | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 14       | 3.14          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 3        | 3.13          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 3        | 3.13          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 3        | 3.13          |
| (1,1074) | 1:866:A:PRO:HD3 | 1:887:A:TYR:HE1  | 17       | 3.12          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 11       | 3.12          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1  | 9        | 3.12          |
| (1,850)  | 1:867:A:TYR:HE1 | 1:870:A:PRO:HA   | 13       | 3.12          |
| (1,1073) | 1:865:A:ALA:HA  | 1:887:A:TYR:HD1  | 16       | 3.11          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 15       | 3.11          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 15       | 3.11          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 15       | 3.11          |
| (1,1073) | 1:865:A:ALA:HA  | 1:887:A:TYR:HD1  | 17       | 3.1           |
| (1,1037) | 1:867:A:TYR:HD2 | 1:878:A:ASP:HB3  | 17       | 3.1           |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1  | 4        | 3.1           |
| (1,1037) | 1:867:A:TYR:HD2 | 1:878:A:ASP:HB3  | 15       | 3.09          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 3        | 3.08          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1  | 2        | 3.08          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG21 | 16       | 3.08          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG22 | 16       | 3.08          |
| (1,400)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG23 | 16       | 3.08          |
| (1,2348) | 1:865:A:ALA:H   | 1:887:A:TYR:HE1  | 16       | 3.07          |
| (1,1037) | 1:867:A:TYR:HD2 | 1:878:A:ASP:HB3  | 16       | 3.07          |
| (1,933)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG11 | 16       | 3.07          |
| (1,933)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG12 | 16       | 3.07          |
| (1,933)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG13 | 16       | 3.07          |
| (1,1035) | 1:867:A:TYR:HD1 | 1:872:A:SER:HB2  | 7        | 3.06          |
| (1,1037) | 1:867:A:TYR:HD2 | 1:878:A:ASP:HB3  | 2        | 3.05          |
| (1,936)  | 1:830:A:MET:HB2 | 1:882:A:PHE:HD1  | 14       | 3.05          |
| (1,1037) | 1:867:A:TYR:HD2 | 1:878:A:ASP:HB3  | 3        | 3.04          |
| (1,1037) | 1:867:A:TYR:HD2 | 1:878:A:ASP:HB3  | 12       | 3.04          |
| (1,933)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG11 | 4        | 3.04          |
| (1,933)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG12 | 4        | 3.04          |
| (1,933)  | 1:771:A:PHE:HD1 | 1:799:A:VAL:HG13 | 4        | 3.04          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 19       | 3.04          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 19       | 3.04          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 19       | 3.04          |
| (1,1037) | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB3  | 8        | 3.03          |
| (1,1037) | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB3  | 14       | 3.03          |
| (1,936)  | 1:830:A:MET:HB2  | 1:882:A:PHE:HD1  | 3        | 3.03          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 2        | 3.03          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 2        | 3.03          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 2        | 3.03          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 13       | 3.03          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 13       | 3.03          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 13       | 3.03          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA   | 13       | 3.03          |
| (1,936)  | 1:830:A:MET:HB2  | 1:882:A:PHE:HD1  | 15       | 3.02          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 17       | 3.02          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 17       | 3.02          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 17       | 3.02          |
| (1,1035) | 1:867:A:TYR:HD1  | 1:872:A:SER:HB2  | 17       | 3.01          |
| (1,1037) | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB3  | 11       | 3.0           |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 19       | 3.0           |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 19       | 3.0           |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 19       | 3.0           |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 7        | 3.0           |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 7        | 3.0           |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 7        | 3.0           |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 18       | 3.0           |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 18       | 3.0           |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 18       | 3.0           |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 19       | 3.0           |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 19       | 3.0           |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 19       | 3.0           |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 1        | 2.99          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 1        | 2.99          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 1        | 2.99          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 5        | 2.99          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 5        | 2.99          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 5        | 2.99          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 14       | 2.99          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 14       | 2.99          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 14       | 2.99          |
| (1,1037) | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB3  | 9        | 2.98          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 13       | 2.98          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 20       | 2.98          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 20       | 2.98          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 20       | 2.98          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 7        | 2.98          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 7        | 2.98          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 7        | 2.98          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 12       | 2.98          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 12       | 2.98          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 12       | 2.98          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 13       | 2.98          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 13       | 2.98          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 13       | 2.98          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 12       | 2.98          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 12       | 2.98          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 12       | 2.98          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 17       | 2.98          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 17       | 2.98          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 17       | 2.98          |
| (1,1037) | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB3  | 6        | 2.97          |
| (1,1037) | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB3  | 13       | 2.97          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 20       | 2.97          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 20       | 2.97          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 20       | 2.97          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA   | 8        | 2.97          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA   | 17       | 2.97          |
| (1,1074) | 1:866:A:PRO:HD3  | 1:887:A:TYR:HE1  | 5        | 2.96          |
| (1,1037) | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB3  | 5        | 2.96          |
| (1,1037) | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB3  | 7        | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 8        | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 8        | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 8        | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 10       | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 10       | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 10       | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 11       | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 11       | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 11       | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 18       | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 18       | 2.96          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 18       | 2.96          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 2        | 2.96          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 2        | 2.96          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 2        | 2.96          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 8        | 2.95          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 19       | 2.95          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 19       | 2.95          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 19       | 2.95          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 9        | 2.95          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 9        | 2.95          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 9        | 2.95          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 1        | 2.95          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 1        | 2.95          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 1        | 2.95          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 6        | 2.95          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 6        | 2.95          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 6        | 2.95          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 16       | 2.95          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 16       | 2.95          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 16       | 2.95          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 6        | 2.94          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 6        | 2.94          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 6        | 2.94          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 20       | 2.94          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 20       | 2.94          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 20       | 2.94          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 4        | 2.94          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 4        | 2.94          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 4        | 2.94          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 10       | 2.94          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 10       | 2.94          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 10       | 2.94          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 17       | 2.92          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 14       | 2.92          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 14       | 2.92          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 14       | 2.92          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 8        | 2.92          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 8        | 2.92          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 8        | 2.92          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA   | 7        | 2.92          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 14       | 2.91          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 14       | 2.91          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 14       | 2.91          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 5        | 2.91          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 5        | 2.91          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 5        | 2.91          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 15       | 2.91          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 15       | 2.91          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 15       | 2.91          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA   | 2        | 2.91          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 6        | 2.9           |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 6        | 2.9           |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 6        | 2.9           |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA   | 8        | 2.9           |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA   | 15       | 2.9           |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 14       | 2.89          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 7        | 2.89          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 7        | 2.89          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 7        | 2.89          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 3        | 2.89          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 3        | 2.89          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 3        | 2.89          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 14       | 2.89          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 14       | 2.89          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 14       | 2.89          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA   | 16       | 2.89          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2  | 17       | 2.88          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3  | 17       | 2.88          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 6        | 2.88          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 11       | 2.88          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG11 | 15       | 2.88          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG12 | 15       | 2.88          |
| (1,933)  | 1:771:A:PHE:HD1  | 1:799:A:VAL:HG13 | 15       | 2.88          |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA   | 2        | 2.88          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA   | 11       | 2.88          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA   | 12       | 2.88          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 2        | 2.87          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 9        | 2.87          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 9        | 2.87          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3  | 9        | 2.87          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA   | 14       | 2.87          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 7        | 2.86          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 9        | 2.86          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 12       | 2.86          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA   | 16       | 2.86          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1  | 11       | 2.86          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2  | 11       | 2.86          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3 | 11       | 2.86          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA  | 3        | 2.86          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA  | 6        | 2.86          |
| (1,936)  | 1:830:A:MET:HB2  | 1:882:A:PHE:HD1 | 1        | 2.85          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB1 | 3        | 2.85          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB2 | 3        | 2.85          |
| (1,932)  | 1:771:A:PHE:HD1  | 1:811:A:ALA:HB3 | 3        | 2.85          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA  | 5        | 2.85          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA  | 15       | 2.84          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1 | 5        | 2.84          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1 | 5        | 2.84          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1 | 5        | 2.84          |
| (1,849)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HA  | 9        | 2.83          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA  | 5        | 2.82          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 20       | 2.82          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 20       | 2.82          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 20       | 2.82          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1 | 18       | 2.82          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1 | 18       | 2.82          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1 | 18       | 2.82          |
| (1,1036) | 1:867:A:TYR:HD1  | 1:872:A:SER:HA  | 3        | 2.81          |
| (1,936)  | 1:830:A:MET:HB2  | 1:882:A:PHE:HD1 | 7        | 2.81          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 6        | 2.79          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 6        | 2.79          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 6        | 2.79          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H   | 10       | 2.78          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 5        | 2.78          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 5        | 2.78          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 5        | 2.78          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 19       | 2.77          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 19       | 2.77          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 19       | 2.77          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1 | 19       | 2.77          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1 | 19       | 2.77          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1 | 19       | 2.77          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H   | 6        | 2.77          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H   | 14       | 2.77          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H   | 15       | 2.77          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H   | 16       | 2.77          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H   | 19       | 2.76          |
| (1,1074) | 1:866:A:PRO:HD3  | 1:887:A:TYR:HE1 | 12       | 2.76          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 7        | 2.75          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 7        | 2.75          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 7        | 2.75          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 12       | 2.74          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 18       | 2.74          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 20       | 2.74          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 3        | 2.74          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 3        | 2.74          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 3        | 2.74          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 5        | 2.73          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 14       | 2.72          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 14       | 2.72          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 14       | 2.72          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 14       | 2.72          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 14       | 2.72          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 14       | 2.72          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 7        | 2.72          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 6        | 2.71          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 6        | 2.71          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 6        | 2.71          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 6        | 2.71          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 6        | 2.71          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 6        | 2.71          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 4        | 2.71          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 8        | 2.71          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 17       | 2.71          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 17       | 2.71          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 17       | 2.71          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 17       | 2.71          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 9        | 2.7           |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 9        | 2.7           |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 9        | 2.7           |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 9        | 2.7           |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 9        | 2.7           |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 9        | 2.7           |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2  | 13       | 2.7           |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 11       | 2.7           |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 4        | 2.7           |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 4        | 2.7           |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 4        | 2.7           |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 5        | 2.69          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 5        | 2.69          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 5        | 2.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 5        | 2.69          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 5        | 2.69          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 5        | 2.69          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 1        | 2.68          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 9        | 2.68          |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA   | 15       | 2.68          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 12       | 2.67          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 12       | 2.67          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 12       | 2.67          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 12       | 2.67          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 12       | 2.67          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 12       | 2.67          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 20       | 2.67          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 20       | 2.67          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 20       | 2.67          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 20       | 2.67          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 20       | 2.67          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 20       | 2.67          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 2        | 2.67          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 1        | 2.67          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 1        | 2.67          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 1        | 2.67          |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2  | 17       | 2.66          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 3        | 2.66          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 13       | 2.66          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 13       | 2.66          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 13       | 2.66          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 18       | 2.65          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 18       | 2.65          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 18       | 2.65          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 8        | 2.65          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 8        | 2.65          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 8        | 2.65          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 13       | 2.65          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 13       | 2.65          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 13       | 2.65          |
| (1,1899) | 1:771:A:PHE:HE1  | 1:812:A:PHE:H    | 13       | 2.64          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 8        | 2.63          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 4        | 2.61          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 4        | 2.61          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 4        | 2.61          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 4        | 2.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 4        | 2.61          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 4        | 2.61          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 3        | 2.61          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 5        | 2.61          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 7        | 2.61          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 13       | 2.61          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 14       | 2.61          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 17       | 2.61          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 17       | 2.61          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 17       | 2.61          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 3        | 2.6           |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 3        | 2.6           |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 3        | 2.6           |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 3        | 2.6           |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 3        | 2.6           |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 3        | 2.6           |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 17       | 2.6           |
| (1,936)  | 1:830:A:MET:HB2  | 1:882:A:PHE:HD1  | 10       | 2.6           |
| (1,936)  | 1:830:A:MET:HB2  | 1:882:A:PHE:HD1  | 18       | 2.6           |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 1        | 2.6           |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 8        | 2.6           |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 8        | 2.6           |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 8        | 2.6           |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 2        | 2.59          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 5        | 2.59          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 11       | 2.59          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 11       | 2.59          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 11       | 2.59          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 7        | 2.58          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 7        | 2.58          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 7        | 2.58          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 9        | 2.57          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 6        | 2.56          |
| (1,1074) | 1:866:A:PRO:HD3  | 1:887:A:TYR:HE1  | 16       | 2.56          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 1        | 2.56          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 1        | 2.56          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 1        | 2.56          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 4        | 2.56          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 4        | 2.56          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 4        | 2.56          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 9        | 2.56          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 9        | 2.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 9        | 2.56          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 13       | 2.56          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 3        | 2.56          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 3        | 2.56          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 3        | 2.56          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 18       | 2.55          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 18       | 2.55          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 18       | 2.55          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 18       | 2.55          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 18       | 2.55          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 18       | 2.55          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 16       | 2.55          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 16       | 2.54          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 11       | 2.54          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 12       | 2.54          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 12       | 2.54          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 12       | 2.54          |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA   | 12       | 2.54          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 15       | 2.53          |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2  | 14       | 2.53          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 2        | 2.53          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 2        | 2.53          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 2        | 2.53          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 19       | 2.53          |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA   | 3        | 2.53          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 11       | 2.52          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 11       | 2.52          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 11       | 2.52          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 14       | 2.52          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 14       | 2.52          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 14       | 2.52          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 15       | 2.52          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 15       | 2.52          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 15       | 2.52          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 2        | 2.51          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 2        | 2.51          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 2        | 2.51          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 2        | 2.51          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 2        | 2.51          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 2        | 2.51          |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2  | 9        | 2.51          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 12       | 2.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 12       | 2.51          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 12       | 2.51          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 15       | 2.51          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 15       | 2.51          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 15       | 2.51          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 5        | 2.51          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 5        | 2.51          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 5        | 2.51          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 16       | 2.51          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 16       | 2.51          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 16       | 2.51          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 6        | 2.5           |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 6        | 2.5           |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 6        | 2.5           |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2  | 6        | 2.49          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 7        | 2.49          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 7        | 2.49          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 7        | 2.49          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 11       | 2.49          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 11       | 2.49          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 11       | 2.49          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 3        | 2.49          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 3        | 2.49          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 3        | 2.49          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 2        | 2.49          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 2        | 2.49          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 2        | 2.49          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 16       | 2.48          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 16       | 2.48          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 16       | 2.48          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 16       | 2.48          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 16       | 2.48          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 16       | 2.48          |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H    | 13       | 2.48          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 8        | 2.48          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 8        | 2.48          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 8        | 2.48          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 12       | 2.48          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 12       | 2.48          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 12       | 2.48          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 8        | 2.48          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 8        | 2.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 8        | 2.48          |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA   | 7        | 2.48          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 12       | 2.47          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 14       | 2.47          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 14       | 2.47          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 14       | 2.47          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 14       | 2.47          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG21 | 9        | 2.47          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG22 | 9        | 2.47          |
| (1,858)  | 1:867:A:TYR:HE1  | 1:873:A:VAL:HG23 | 9        | 2.47          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 1        | 2.46          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 1        | 2.46          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 1        | 2.46          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 1        | 2.46          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 1        | 2.46          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 1        | 2.46          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 7        | 2.46          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 7        | 2.46          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 7        | 2.46          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 7        | 2.46          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 7        | 2.46          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 7        | 2.46          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 5        | 2.46          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 5        | 2.46          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 5        | 2.46          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 6        | 2.46          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 6        | 2.46          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 6        | 2.46          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 20       | 2.46          |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2  | 2        | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 3        | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 3        | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 3        | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 9        | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 9        | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 9        | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 13       | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 13       | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 13       | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 16       | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 16       | 2.45          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 16       | 2.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 15       | 2.45          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 15       | 2.45          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 15       | 2.45          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 10       | 2.45          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 6        | 2.44          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 17       | 2.44          |
| (1,2396) | 1:867:A:TYR:HD1  | 1:876:A:ALA:H    | 11       | 2.43          |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA   | 16       | 2.43          |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA   | 17       | 2.43          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2  | 3        | 2.43          |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2  | 12       | 2.42          |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2  | 8        | 2.41          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 15       | 2.41          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 15       | 2.41          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 15       | 2.41          |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA   | 5        | 2.4           |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 8        | 2.39          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 8        | 2.39          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 8        | 2.39          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 8        | 2.39          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1  | 8        | 2.39          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1  | 8        | 2.39          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG21 | 2        | 2.39          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG22 | 2        | 2.39          |
| (1,1041) | 1:867:A:TYR:HD1  | 1:873:A:VAL:HG23 | 2        | 2.39          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 7        | 2.38          |
| (1,1072) | 1:886:A:LEU:HA   | 1:887:A:TYR:HD1  | 17       | 2.37          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 3        | 2.37          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2  | 18       | 2.37          |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2  | 11       | 2.35          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 4        | 2.35          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 9        | 2.34          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 9        | 2.34          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 9        | 2.34          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 11       | 2.34          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 11       | 2.34          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 11       | 2.34          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2  | 9        | 2.34          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 15       | 2.33          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 15       | 2.33          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 15       | 2.33          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1  | 15       | 2.33          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1 | 15       | 2.33          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1 | 15       | 2.33          |
| (1,1072) | 1:886:A:LEU:HA   | 1:887:A:TYR:HD1 | 3        | 2.33          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 13       | 2.33          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 13       | 2.33          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 13       | 2.33          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 4        | 2.33          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 4        | 2.33          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 4        | 2.33          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 6        | 2.33          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 6        | 2.33          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 6        | 2.33          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 10       | 2.33          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 10       | 2.33          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 10       | 2.33          |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA  | 9        | 2.33          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1 | 10       | 2.32          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1 | 10       | 2.32          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1 | 10       | 2.32          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 1        | 2.32          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 1        | 2.32          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 1        | 2.32          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 14       | 2.32          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 14       | 2.32          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 14       | 2.32          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 9        | 2.32          |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2 | 7        | 2.31          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 17       | 2.31          |
| (1,1072) | 1:886:A:LEU:HA   | 1:887:A:TYR:HD1 | 5        | 2.31          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 3        | 2.31          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 3        | 2.31          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 3        | 2.31          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 5        | 2.31          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 5        | 2.31          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 5        | 2.31          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 15       | 2.31          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 15       | 2.31          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 15       | 2.31          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2 | 15       | 2.31          |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA  | 6        | 2.31          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 2        | 2.31          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 4        | 2.31          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 13       | 2.3           |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 2        | 2.3           |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 2        | 2.3           |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 2        | 2.3           |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1 | 16       | 2.3           |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1 | 16       | 2.3           |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1 | 16       | 2.3           |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2 | 12       | 2.3           |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA  | 11       | 2.3           |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2 | 15       | 2.29          |
| (1,1072) | 1:886:A:LEU:HA   | 1:887:A:TYR:HD1 | 18       | 2.29          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 18       | 2.29          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 18       | 2.29          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 18       | 2.29          |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2 | 5        | 2.28          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 11       | 2.28          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 11       | 2.28          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 11       | 2.28          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 9        | 2.28          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 9        | 2.28          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 9        | 2.28          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 11       | 2.28          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 11       | 2.28          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 11       | 2.28          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2 | 2        | 2.28          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 13       | 2.28          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 16       | 2.28          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 13       | 2.27          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 13       | 2.27          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 13       | 2.27          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1 | 13       | 2.27          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1 | 13       | 2.27          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1 | 13       | 2.27          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 12       | 2.27          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 12       | 2.27          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 12       | 2.27          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 2        | 2.27          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 2        | 2.27          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 2        | 2.27          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 19       | 2.27          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 19       | 2.27          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 19       | 2.27          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 20       | 2.27          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 20       | 2.27          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 20       | 2.27          |
| (1,850)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HA  | 14       | 2.27          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 1        | 2.27          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 7        | 2.27          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 11       | 2.26          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 11       | 2.26          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 11       | 2.26          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1 | 11       | 2.26          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1 | 11       | 2.26          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1 | 11       | 2.26          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 16       | 2.26          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 8        | 2.26          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 8        | 2.26          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 8        | 2.26          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 12       | 2.26          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 12       | 2.26          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 12       | 2.26          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 16       | 2.26          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 16       | 2.26          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 16       | 2.26          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 17       | 2.26          |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2 | 16       | 2.25          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 7        | 2.25          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 7        | 2.25          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 7        | 2.25          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 5        | 2.25          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 14       | 2.25          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 15       | 2.25          |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 13       | 2.24          |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 13       | 2.24          |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 13       | 2.24          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 6        | 2.24          |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2 | 8        | 2.23          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 19       | 2.22          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 19       | 2.22          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 19       | 2.22          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 19       | 2.22          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 19       | 2.22          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 19       | 2.22          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 2        | 2.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 13       | 2.22          |
| (1,1072) | 1:886:A:LEU:HA   | 1:887:A:TYR:HD1 | 12       | 2.22          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 19       | 2.21          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 8        | 2.21          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 10       | 2.21          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 15       | 2.2           |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 7        | 2.2           |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 12       | 2.2           |
| (1,890)  | 1:766:A:LEU:HD21 | 1:771:A:PHE:HD2 | 17       | 2.2           |
| (1,890)  | 1:766:A:LEU:HD22 | 1:771:A:PHE:HD2 | 17       | 2.2           |
| (1,890)  | 1:766:A:LEU:HD23 | 1:771:A:PHE:HD2 | 17       | 2.2           |
| (1,886)  | 1:770:A:GLU:HB3  | 1:771:A:PHE:HD2 | 18       | 2.2           |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 12       | 2.2           |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 6        | 2.19          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 11       | 2.19          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 20       | 2.19          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 19       | 2.19          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 3        | 2.18          |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H   | 8        | 2.18          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 11       | 2.18          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 2        | 2.17          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 8        | 2.17          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 18       | 2.17          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 11       | 2.17          |
| (1,133)  | 1:766:A:LEU:HG   | 1:771:A:PHE:HD2 | 20       | 2.17          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 8        | 2.16          |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H   | 2        | 2.16          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 14       | 2.15          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 14       | 2.15          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 14       | 2.15          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 14       | 2.15          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 14       | 2.15          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 14       | 2.15          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 5        | 2.14          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 12       | 2.14          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 17       | 2.14          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 1        | 2.14          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 16       | 2.14          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 10       | 2.14          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 10       | 2.14          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 10       | 2.14          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2 | 8        | 2.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3 | 8        | 2.13          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 9        | 2.13          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 5        | 2.13          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 7        | 2.12          |
| (1,2409) | 1:867:A:TYR:HD2  | 1:878:A:ASP:H   | 14       | 2.12          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 20       | 2.11          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 20       | 2.11          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 20       | 2.11          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 20       | 2.11          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 20       | 2.11          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 20       | 2.11          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 6        | 2.1           |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1 | 15       | 2.1           |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1 | 15       | 2.1           |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1 | 15       | 2.1           |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1 | 17       | 2.1           |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1 | 17       | 2.1           |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1 | 17       | 2.1           |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 17       | 2.08          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 17       | 2.08          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 17       | 2.08          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1 | 17       | 2.08          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1 | 17       | 2.08          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1 | 17       | 2.08          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 9        | 2.08          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 10       | 2.08          |
| (1,2640) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 10       | 2.07          |
| (1,2640) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 10       | 2.07          |
| (1,2640) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 10       | 2.07          |
| (1,2640) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1 | 10       | 2.07          |
| (1,2640) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1 | 10       | 2.07          |
| (1,2640) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1 | 10       | 2.07          |
| (1,2093) | 1:841:A:ASN:HD21 | 1:867:A:TYR:HE2 | 3        | 2.07          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 15       | 2.07          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 14       | 2.06          |
| (1,941)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HD1 | 17       | 2.06          |
| (1,941)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HD1 | 17       | 2.06          |
| (1,941)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HD1 | 17       | 2.06          |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA2 | 16       | 2.05          |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA3 | 16       | 2.05          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 3        | 2.05          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 5        | 2.04          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 5        | 2.04          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 5        | 2.04          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 5        | 2.04          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 5        | 2.04          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 5        | 2.04          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 6        | 2.04          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 6        | 2.04          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 6        | 2.04          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 6        | 2.04          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 6        | 2.04          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 6        | 2.04          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 12       | 2.04          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 12       | 2.04          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 12       | 2.04          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 12       | 2.04          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 12       | 2.04          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 12       | 2.04          |
| (1,1823) | 1:771:A:PHE:HD1  | 1:808:A:THR:H   | 4        | 2.04          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 1        | 2.04          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 1        | 2.04          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 1        | 2.04          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 13       | 2.03          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 13       | 2.03          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 13       | 2.03          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2 | 4        | 2.02          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3 | 4        | 2.02          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 16       | 2.01          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 16       | 2.01          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 16       | 2.01          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1 | 3        | 2.01          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1 | 3        | 2.01          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1 | 3        | 2.01          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 7        | 2.01          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 7        | 2.01          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 7        | 2.01          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 19       | 2.01          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 19       | 2.01          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 19       | 2.01          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 14       | 2.01          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 14       | 2.01          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 14       | 2.01          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 12       | 2.0           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 12       | 2.0           |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 12       | 2.0           |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 18       | 2.0           |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 18       | 2.0           |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 18       | 2.0           |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 9        | 2.0           |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 9        | 2.0           |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 9        | 2.0           |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 18       | 2.0           |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 18       | 2.0           |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 18       | 2.0           |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2 | 12       | 1.99          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3 | 12       | 1.99          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 9        | 1.99          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 9        | 1.99          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 9        | 1.99          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 16       | 1.99          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 16       | 1.99          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 16       | 1.99          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 20       | 1.99          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 20       | 1.99          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 20       | 1.99          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 10       | 1.98          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 10       | 1.98          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 10       | 1.98          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 5        | 1.98          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 5        | 1.98          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 5        | 1.98          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 6        | 1.97          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 6        | 1.97          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 6        | 1.97          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 17       | 1.97          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 17       | 1.97          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 17       | 1.97          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 3        | 1.97          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 3        | 1.97          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 3        | 1.97          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 4        | 1.97          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 4        | 1.97          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 4        | 1.97          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 12       | 1.96          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 12       | 1.96          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 12       | 1.96          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 2        | 1.96          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 2        | 1.96          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 2        | 1.96          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 6        | 1.96          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 6        | 1.96          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 6        | 1.96          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 8        | 1.95          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 8        | 1.95          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 8        | 1.95          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 14       | 1.95          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 14       | 1.95          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 14       | 1.95          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 7        | 1.95          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 7        | 1.95          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 7        | 1.95          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 10       | 1.95          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 10       | 1.95          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 10       | 1.95          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 19       | 1.95          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 19       | 1.95          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 19       | 1.95          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 9        | 1.94          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 9        | 1.94          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 9        | 1.94          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 9        | 1.94          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 9        | 1.94          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 9        | 1.94          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 4        | 1.94          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 4        | 1.94          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 4        | 1.94          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 15       | 1.94          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 15       | 1.94          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 15       | 1.94          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 1        | 1.93          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 1        | 1.93          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 1        | 1.93          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 5        | 1.93          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 5        | 1.93          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 5        | 1.93          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 2        | 1.93          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 2        | 1.93          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 2        | 1.93          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 15       | 1.92          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 15       | 1.92          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 15       | 1.92          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 19       | 1.91          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 19       | 1.91          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 19       | 1.91          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 8        | 1.91          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 8        | 1.91          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 8        | 1.91          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1 | 9        | 1.9           |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1 | 9        | 1.9           |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1 | 9        | 1.9           |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 11       | 1.9           |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 11       | 1.9           |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 11       | 1.9           |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 20       | 1.9           |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 20       | 1.9           |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 20       | 1.9           |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 4        | 1.89          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 4        | 1.89          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 4        | 1.89          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 4        | 1.89          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 4        | 1.89          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 4        | 1.89          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1 | 12       | 1.89          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1 | 12       | 1.89          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1 | 12       | 1.89          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1 | 18       | 1.89          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1 | 18       | 1.89          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1 | 18       | 1.89          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 9        | 1.89          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 9        | 1.89          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 9        | 1.89          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 12       | 1.88          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 12       | 1.88          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 12       | 1.88          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 13       | 1.88          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 13       | 1.88          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 13       | 1.88          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 11       | 1.87          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 11       | 1.87          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 11       | 1.87          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 16       | 1.86          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 16       | 1.86          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 16       | 1.86          |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H   | 15       | 1.85          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 14       | 1.85          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 14       | 1.85          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 14       | 1.85          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 5        | 1.84          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 5        | 1.84          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 5        | 1.84          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2 | 5        | 1.83          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3 | 5        | 1.83          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 2        | 1.83          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 2        | 1.83          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 2        | 1.83          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 2        | 1.83          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 2        | 1.83          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 2        | 1.83          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 6        | 1.83          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 6        | 1.83          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 6        | 1.83          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB1 | 3        | 1.83          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB2 | 3        | 1.83          |
| (1,935)  | 1:771:A:PHE:HE1  | 1:811:A:ALA:HB3 | 3        | 1.83          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 3        | 1.81          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 3        | 1.81          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 3        | 1.81          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 3        | 1.81          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 3        | 1.81          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 3        | 1.81          |
| (1,1072) | 1:886:A:LEU:HA   | 1:887:A:TYR:HD1 | 16       | 1.81          |
| (1,761)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HD2 | 17       | 1.81          |
| (1,761)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HD2 | 17       | 1.81          |
| (1,761)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HD2 | 17       | 1.81          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 7        | 1.78          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 7        | 1.78          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 7        | 1.78          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 7        | 1.78          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 7        | 1.78          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 7        | 1.78          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 18       | 1.77          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 18       | 1.77          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 18       | 1.77          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 18       | 1.77          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 18       | 1.77          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 18       | 1.77          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 4        | 1.77          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 4        | 1.77          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 4        | 1.77          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 1        | 1.76          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 1        | 1.76          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 1        | 1.76          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 1        | 1.76          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 1        | 1.76          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 1        | 1.76          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 20       | 1.76          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 20       | 1.76          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 20       | 1.76          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1 | 2        | 1.76          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1 | 2        | 1.76          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1 | 2        | 1.76          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 12       | 1.76          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 12       | 1.76          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 12       | 1.76          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 19       | 1.76          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 19       | 1.76          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 19       | 1.76          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 15       | 1.75          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 15       | 1.75          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 15       | 1.75          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 15       | 1.75          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 15       | 1.75          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 15       | 1.75          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 16       | 1.75          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 16       | 1.75          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 16       | 1.75          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 16       | 1.75          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 16       | 1.75          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 16       | 1.75          |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3 | 13       | 1.75          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 3        | 1.74          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 3        | 1.74          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 3        | 1.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 16       | 1.74          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 16       | 1.74          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 16       | 1.74          |
| (1,989)  | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 17       | 1.72          |
| (1,989)  | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 17       | 1.72          |
| (1,989)  | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 17       | 1.72          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 2        | 1.68          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 2        | 1.68          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 2        | 1.68          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 14       | 1.67          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 14       | 1.67          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 14       | 1.67          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 18       | 1.64          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 18       | 1.64          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 18       | 1.64          |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3  | 6        | 1.64          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 11       | 1.63          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 11       | 1.63          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 11       | 1.63          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 11       | 1.63          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 11       | 1.63          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 11       | 1.63          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 6        | 1.63          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 6        | 1.63          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 6        | 1.63          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 17       | 1.63          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 17       | 1.63          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 17       | 1.63          |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3  | 15       | 1.63          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 20       | 1.63          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 20       | 1.63          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 20       | 1.63          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 13       | 1.62          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 13       | 1.62          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 13       | 1.62          |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3  | 17       | 1.62          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 18       | 1.61          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 18       | 1.61          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 18       | 1.61          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 8        | 1.6           |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 8        | 1.6           |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 8        | 1.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 8        | 1.6           |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 8        | 1.6           |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 8        | 1.6           |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 16       | 1.6           |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 16       | 1.6           |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 16       | 1.6           |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 13       | 1.59          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 13       | 1.59          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 13       | 1.59          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1  | 13       | 1.59          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1  | 13       | 1.59          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1  | 13       | 1.59          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 7        | 1.58          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 7        | 1.58          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 7        | 1.58          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 19       | 1.58          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 19       | 1.58          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 19       | 1.58          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 20       | 1.57          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 20       | 1.57          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 20       | 1.57          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 1        | 1.57          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 1        | 1.57          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 1        | 1.57          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 12       | 1.57          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 12       | 1.57          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 12       | 1.57          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 2        | 1.56          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 2        | 1.56          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 2        | 1.56          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 7        | 1.56          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 7        | 1.56          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 7        | 1.56          |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2  | 13       | 1.56          |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3  | 9        | 1.56          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 9        | 1.56          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 9        | 1.56          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 9        | 1.56          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 1        | 1.55          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 1        | 1.55          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 1        | 1.55          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 11       | 1.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 11       | 1.55          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 11       | 1.55          |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3  | 2        | 1.55          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 5        | 1.55          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 5        | 1.55          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 5        | 1.55          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 6        | 1.55          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 6        | 1.55          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 6        | 1.55          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2  | 3        | 1.54          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3  | 3        | 1.54          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 14       | 1.54          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 14       | 1.54          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 14       | 1.54          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 8        | 1.54          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 8        | 1.54          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 8        | 1.54          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 10       | 1.54          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 19       | 1.53          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 19       | 1.53          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 19       | 1.53          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 3        | 1.53          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 3        | 1.53          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 3        | 1.53          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 20       | 1.53          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 20       | 1.53          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 20       | 1.53          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 4        | 1.52          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 4        | 1.52          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 4        | 1.52          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 5        | 1.51          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 5        | 1.51          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 5        | 1.51          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 15       | 1.51          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 15       | 1.51          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 15       | 1.51          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 3        | 1.51          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 6        | 1.51          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 14       | 1.5           |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 14       | 1.5           |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 14       | 1.5           |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3  | 14       | 1.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 15       | 1.5           |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 9        | 1.49          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 9        | 1.49          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 9        | 1.49          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 10       | 1.49          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 10       | 1.49          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 10       | 1.49          |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3  | 3        | 1.49          |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3  | 8        | 1.49          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 1        | 1.49          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 14       | 1.49          |
| (1,2716) | 1:887:A:TYR:HE2  | 1:888:A:GLY:HA2  | 16       | 1.48          |
| (1,2716) | 1:887:A:TYR:HE2  | 1:888:A:GLY:HA3  | 16       | 1.48          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2  | 11       | 1.48          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3  | 11       | 1.48          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 7        | 1.48          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 7        | 1.48          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 7        | 1.48          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 6        | 1.48          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 6        | 1.48          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 6        | 1.48          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 4        | 1.48          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2  | 16       | 1.47          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3  | 16       | 1.47          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 4        | 1.47          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 4        | 1.47          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 4        | 1.47          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG11 | 16       | 1.47          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG12 | 16       | 1.47          |
| (1,891)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG13 | 16       | 1.47          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 5        | 1.47          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 16       | 1.47          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 18       | 1.47          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 19       | 1.47          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2  | 17       | 1.46          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3  | 11       | 1.46          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2  | 16       | 1.45          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 8        | 1.45          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 8        | 1.45          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 8        | 1.45          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 1        | 1.45          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 1        | 1.45          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1 | 1        | 1.45          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3 | 12       | 1.45          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2 | 10       | 1.44          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3 | 2        | 1.44          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3 | 9        | 1.44          |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H   | 13       | 1.43          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2 | 8        | 1.43          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1 | 13       | 1.43          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1 | 13       | 1.43          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1 | 13       | 1.43          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3 | 8        | 1.43          |
| (1,778)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HB3 | 13       | 1.42          |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3 | 11       | 1.42          |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3 | 16       | 1.42          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3 | 7        | 1.42          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3 | 20       | 1.42          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2 | 4        | 1.41          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 15       | 1.41          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 15       | 1.41          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 15       | 1.41          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3 | 13       | 1.41          |
| (1,491)  | 1:771:A:PHE:HD1  | 1:812:A:PHE:HB3 | 17       | 1.41          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2 | 11       | 1.4           |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2 | 12       | 1.4           |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3 | 5        | 1.4           |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 2        | 1.4           |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 2        | 1.4           |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 2        | 1.4           |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 4        | 1.4           |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 4        | 1.4           |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 4        | 1.4           |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 16       | 1.4           |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 16       | 1.4           |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 16       | 1.4           |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3 | 12       | 1.39          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2 | 18       | 1.38          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2 | 18       | 1.36          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3 | 18       | 1.36          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2 | 19       | 1.36          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3 | 19       | 1.36          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2 | 5        | 1.36          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1 | 5        | 1.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 5        | 1.36          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 5        | 1.36          |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2  | 8        | 1.36          |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA2  | 5        | 1.35          |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA3  | 5        | 1.35          |
| (1,778)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HB3  | 17       | 1.35          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 17       | 1.35          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 17       | 1.35          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 17       | 1.35          |
| (1,1644) | 1:792:A:PHE:H    | 1:794:A:ARG:HG2  | 11       | 1.34          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2  | 20       | 1.34          |
| (1,778)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HB3  | 6        | 1.34          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 13       | 1.34          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 13       | 1.34          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 13       | 1.34          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2  | 1        | 1.33          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2  | 3        | 1.33          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2  | 9        | 1.33          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2  | 13       | 1.33          |
| (1,778)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HB3  | 15       | 1.33          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2  | 13       | 1.32          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3  | 13       | 1.32          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2  | 15       | 1.32          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 11       | 1.32          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 11       | 1.32          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 11       | 1.32          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 8        | 1.32          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 8        | 1.32          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 8        | 1.32          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 7        | 1.32          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 7        | 1.32          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 7        | 1.32          |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA2  | 3        | 1.31          |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA3  | 3        | 1.31          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2  | 6        | 1.31          |
| (1,940)  | 1:830:A:MET:HE1  | 1:882:A:PHE:HD1  | 10       | 1.31          |
| (1,940)  | 1:830:A:MET:HE2  | 1:882:A:PHE:HD1  | 10       | 1.31          |
| (1,940)  | 1:830:A:MET:HE3  | 1:882:A:PHE:HD1  | 10       | 1.31          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 13       | 1.31          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 13       | 1.31          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 13       | 1.31          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 3        | 1.31          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 3        | 1.31          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 3        | 1.31          |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA2 | 12       | 1.3           |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA3 | 12       | 1.3           |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2 | 1        | 1.3           |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3 | 1        | 1.3           |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2 | 7        | 1.3           |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2 | 14       | 1.3           |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2 | 6        | 1.29          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3 | 6        | 1.29          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2 | 2        | 1.29          |
| (1,984)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HE2 | 19       | 1.29          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 10       | 1.28          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 10       | 1.28          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 10       | 1.28          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 10       | 1.28          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 10       | 1.28          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 10       | 1.28          |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1 | 13       | 1.28          |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1 | 13       | 1.28          |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1 | 13       | 1.28          |
| (1,777)  | 1:867:A:TYR:HD1  | 1:872:A:SER:HB3 | 7        | 1.28          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2 | 10       | 1.27          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3 | 10       | 1.27          |
| (1,973)  | 1:771:A:PHE:HE1  | 1:812:A:PHE:HD2 | 10       | 1.26          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1 | 3        | 1.26          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2 | 3        | 1.26          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3 | 3        | 1.26          |
| (1,778)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HB3 | 9        | 1.26          |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA2 | 17       | 1.25          |
| (1,2717) | 1:887:A:TYR:HD2  | 1:888:A:GLY:HA3 | 17       | 1.25          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2 | 15       | 1.25          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3 | 15       | 1.25          |
| (1,2641) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 17       | 1.25          |
| (1,2641) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 17       | 1.25          |
| (1,2641) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 17       | 1.25          |
| (1,2641) | 1:829:A:VAL:HG21 | 1:882:A:PHE:HE1 | 17       | 1.25          |
| (1,2641) | 1:829:A:VAL:HG22 | 1:882:A:PHE:HE1 | 17       | 1.25          |
| (1,2641) | 1:829:A:VAL:HG23 | 1:882:A:PHE:HE1 | 17       | 1.25          |
| (1,973)  | 1:771:A:PHE:HE1  | 1:812:A:PHE:HD2 | 14       | 1.25          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1 | 8        | 1.25          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2 | 8        | 1.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 8        | 1.25          |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2  | 2        | 1.25          |
| (1,778)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HB3  | 3        | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 2        | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 2        | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 2        | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 8        | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 8        | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 8        | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 12       | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 12       | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 12       | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 16       | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 16       | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 16       | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 19       | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 19       | 1.25          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 19       | 1.25          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2  | 20       | 1.24          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3  | 20       | 1.24          |
| (1,1644) | 1:792:A:PHE:H    | 1:794:A:ARG:HG2  | 3        | 1.24          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 17       | 1.24          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 17       | 1.24          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 17       | 1.24          |
| (1,778)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HB3  | 2        | 1.24          |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H    | 8        | 1.23          |
| (1,973)  | 1:771:A:PHE:HE1  | 1:812:A:PHE:HD2  | 15       | 1.23          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 11       | 1.23          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 11       | 1.23          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 11       | 1.23          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 15       | 1.23          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 15       | 1.23          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 15       | 1.23          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 20       | 1.23          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 20       | 1.23          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 20       | 1.23          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2  | 9        | 1.22          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3  | 9        | 1.22          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 2        | 1.22          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 2        | 1.22          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 2        | 1.22          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 7        | 1.22          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 7        | 1.22          |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 7        | 1.22          |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 14       | 1.22          |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 14       | 1.22          |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 14       | 1.22          |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 16       | 1.22          |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 16       | 1.22          |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 16       | 1.22          |
| (1,855) | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2  | 3        | 1.22          |
| (1,778) | 1:867:A:TYR:HE1  | 1:872:A:SER:HB3  | 14       | 1.22          |
| (1,554) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 1        | 1.22          |
| (1,554) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 1        | 1.22          |
| (1,554) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 1        | 1.22          |
| (1,554) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 18       | 1.22          |
| (1,554) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 18       | 1.22          |
| (1,554) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 18       | 1.22          |
| (1,439) | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 9        | 1.22          |
| (1,439) | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 9        | 1.22          |
| (1,439) | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 9        | 1.22          |
| (1,973) | 1:771:A:PHE:HE1  | 1:812:A:PHE:HD2  | 6        | 1.21          |
| (1,973) | 1:771:A:PHE:HE1  | 1:812:A:PHE:HD2  | 16       | 1.21          |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 5        | 1.21          |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 5        | 1.21          |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 5        | 1.21          |
| (1,855) | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2  | 15       | 1.21          |
| (1,554) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 7        | 1.21          |
| (1,554) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 7        | 1.21          |
| (1,554) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 7        | 1.21          |
| (1,439) | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 6        | 1.21          |
| (1,439) | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 6        | 1.21          |
| (1,439) | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 6        | 1.21          |
| (1,439) | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 18       | 1.21          |
| (1,439) | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 18       | 1.21          |
| (1,439) | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 18       | 1.21          |
| (1,973) | 1:771:A:PHE:HE1  | 1:812:A:PHE:HD2  | 5        | 1.2           |
| (1,942) | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 17       | 1.2           |
| (1,942) | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 17       | 1.2           |
| (1,942) | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 17       | 1.2           |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 12       | 1.2           |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 12       | 1.2           |
| (1,857) | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 12       | 1.2           |
| (1,439) | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 1        | 1.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG22 | 1        | 1.2           |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG23 | 1        | 1.2           |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG21 | 4        | 1.2           |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG22 | 4        | 1.2           |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG23 | 4        | 1.2           |
| (1,1644) | 1:792:A:PHE:H   | 1:794:A:ARG:HG2  | 6        | 1.19          |
| (1,973)  | 1:771:A:PHE:HE1 | 1:812:A:PHE:HD2  | 19       | 1.19          |
| (1,857)  | 1:867:A:TYR:HE1 | 1:876:A:ALA:HB1  | 6        | 1.19          |
| (1,857)  | 1:867:A:TYR:HE1 | 1:876:A:ALA:HB2  | 6        | 1.19          |
| (1,857)  | 1:867:A:TYR:HE1 | 1:876:A:ALA:HB3  | 6        | 1.19          |
| (1,778)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB3  | 8        | 1.19          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG21 | 5        | 1.19          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG22 | 5        | 1.19          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG23 | 5        | 1.19          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG21 | 10       | 1.19          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG22 | 10       | 1.19          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG23 | 10       | 1.19          |
| (1,973)  | 1:771:A:PHE:HE1 | 1:812:A:PHE:HD2  | 3        | 1.18          |
| (1,973)  | 1:771:A:PHE:HE1 | 1:812:A:PHE:HD2  | 8        | 1.18          |
| (1,973)  | 1:771:A:PHE:HE1 | 1:812:A:PHE:HD2  | 9        | 1.18          |
| (1,973)  | 1:771:A:PHE:HE1 | 1:812:A:PHE:HD2  | 18       | 1.18          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG21 | 11       | 1.18          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG22 | 11       | 1.18          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG23 | 11       | 1.18          |
| (1,973)  | 1:771:A:PHE:HE1 | 1:812:A:PHE:HD2  | 1        | 1.17          |
| (1,973)  | 1:771:A:PHE:HE1 | 1:812:A:PHE:HD2  | 12       | 1.17          |
| (1,973)  | 1:771:A:PHE:HE1 | 1:812:A:PHE:HD2  | 20       | 1.17          |
| (1,855)  | 1:867:A:TYR:HE1 | 1:870:A:PRO:HG2  | 12       | 1.17          |
| (1,2717) | 1:887:A:TYR:HD2 | 1:888:A:GLY:HA2  | 18       | 1.16          |
| (1,2717) | 1:887:A:TYR:HD2 | 1:888:A:GLY:HA3  | 18       | 1.16          |
| (1,778)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB3  | 5        | 1.16          |
| (1,778)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB3  | 12       | 1.16          |
| (1,778)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB3  | 16       | 1.16          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG21 | 15       | 1.16          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG22 | 15       | 1.16          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG23 | 15       | 1.16          |
| (1,973)  | 1:771:A:PHE:HE1 | 1:812:A:PHE:HD2  | 2        | 1.15          |
| (1,973)  | 1:771:A:PHE:HE1 | 1:812:A:PHE:HD2  | 4        | 1.15          |
| (1,778)  | 1:867:A:TYR:HE1 | 1:872:A:SER:HB3  | 11       | 1.15          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG21 | 3        | 1.15          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG22 | 3        | 1.15          |
| (1,439)  | 1:771:A:PHE:HD1 | 1:807:A:VAL:HG23 | 3        | 1.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG21 | 14       | 1.15          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG22 | 14       | 1.15          |
| (1,439)  | 1:771:A:PHE:HD1  | 1:807:A:VAL:HG23 | 14       | 1.15          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 15       | 1.14          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 15       | 1.14          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 15       | 1.14          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1  | 17       | 1.13          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2  | 17       | 1.13          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3  | 17       | 1.13          |
| (1,973)  | 1:771:A:PHE:HE1  | 1:812:A:PHE:HD2  | 11       | 1.12          |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H    | 2        | 1.11          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB1  | 9        | 1.11          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB2  | 9        | 1.11          |
| (1,857)  | 1:867:A:TYR:HE1  | 1:876:A:ALA:HB3  | 9        | 1.11          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 11       | 1.11          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 11       | 1.11          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 11       | 1.11          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2  | 14       | 1.1           |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3  | 14       | 1.1           |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1  | 13       | 1.1           |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2  | 13       | 1.1           |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3  | 13       | 1.1           |
| (1,942)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HD1  | 10       | 1.1           |
| (1,942)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HD1  | 10       | 1.1           |
| (1,942)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HD1  | 10       | 1.1           |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2  | 2        | 1.09          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3  | 2        | 1.09          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H    | 19       | 1.09          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1  | 3        | 1.09          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2  | 3        | 1.09          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3  | 3        | 1.09          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1  | 12       | 1.09          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2  | 12       | 1.09          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3  | 12       | 1.09          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1  | 14       | 1.09          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2  | 14       | 1.09          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3  | 14       | 1.09          |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2  | 17       | 1.09          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H    | 2        | 1.08          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H    | 6        | 1.08          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1  | 5        | 1.08          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2  | 5        | 1.08          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3 | 5        | 1.08          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1 | 7        | 1.08          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2 | 7        | 1.08          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3 | 7        | 1.08          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1 | 8        | 1.08          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2 | 8        | 1.08          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3 | 8        | 1.08          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1 | 16       | 1.08          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2 | 16       | 1.08          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3 | 16       | 1.08          |
| (1,973)  | 1:771:A:PHE:HE1  | 1:812:A:PHE:HD2 | 7        | 1.08          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 14       | 1.07          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1 | 6        | 1.07          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2 | 6        | 1.07          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3 | 6        | 1.07          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1 | 11       | 1.07          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2 | 11       | 1.07          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3 | 11       | 1.07          |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2 | 7        | 1.07          |
| (1,778)  | 1:867:A:TYR:HE1  | 1:872:A:SER:HB3 | 7        | 1.07          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1 | 10       | 1.07          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1 | 10       | 1.07          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1 | 10       | 1.07          |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H   | 3        | 1.06          |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2 | 16       | 1.06          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2 | 17       | 1.05          |
| (1,973)  | 1:771:A:PHE:HE1  | 1:812:A:PHE:HD2 | 17       | 1.05          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 13       | 1.05          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 13       | 1.05          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 13       | 1.05          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 11       | 1.04          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2 | 13       | 1.04          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1 | 2        | 1.04          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2 | 2        | 1.04          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3 | 2        | 1.04          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1 | 9        | 1.04          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2 | 9        | 1.04          |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3 | 9        | 1.04          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 13       | 1.03          |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H   | 17       | 1.03          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 8        | 1.03          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 8        | 1.03          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 8        | 1.03          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 10       | 1.03          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 10       | 1.03          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 10       | 1.03          |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2 | 11       | 1.02          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2 | 9        | 1.02          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 15       | 1.02          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 6        | 1.02          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 6        | 1.02          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 6        | 1.02          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 11       | 1.02          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 11       | 1.02          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 11       | 1.02          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 18       | 1.02          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 18       | 1.02          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 18       | 1.02          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 19       | 1.02          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 19       | 1.02          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 19       | 1.02          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 17       | 1.01          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 1        | 1.01          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 1        | 1.01          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 1        | 1.01          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 4        | 1.01          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 4        | 1.01          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 4        | 1.01          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 9        | 1.0           |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H   | 6        | 1.0           |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB1 | 15       | 1.0           |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB2 | 15       | 1.0           |
| (1,1040) | 1:867:A:TYR:HD1  | 1:876:A:ALA:HB3 | 15       | 1.0           |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 5        | 1.0           |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 5        | 1.0           |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 5        | 1.0           |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 14       | 1.0           |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 14       | 1.0           |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 14       | 1.0           |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 20       | 1.0           |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 20       | 1.0           |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 20       | 1.0           |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 7        | 0.99          |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2 | 5        | 0.99          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 2        | 0.99          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 2        | 0.99          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 2        | 0.99          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 15       | 0.99          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 15       | 0.99          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 15       | 0.99          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 15       | 0.98          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 2        | 0.98          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 12       | 0.98          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 3        | 0.98          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 3        | 0.98          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 3        | 0.98          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 12       | 0.98          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 12       | 0.98          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 12       | 0.98          |
| (1,2494) | 1:887:A:TYR:H    | 1:887:A:TYR:HE1 | 17       | 0.97          |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H   | 12       | 0.97          |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H   | 15       | 0.97          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 8        | 0.97          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 7        | 0.97          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 7        | 0.97          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 7        | 0.97          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 8        | 0.97          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 8        | 0.97          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 8        | 0.97          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 9        | 0.97          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 9        | 0.97          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 9        | 0.97          |
| (1,2494) | 1:887:A:TYR:H    | 1:887:A:TYR:HE1 | 18       | 0.96          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 1        | 0.96          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 3        | 0.96          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 13       | 0.96          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 13       | 0.96          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 13       | 0.96          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 16       | 0.96          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 16       | 0.96          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 16       | 0.96          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2 | 13       | 0.95          |
| (1,2494) | 1:887:A:TYR:H    | 1:887:A:TYR:HE1 | 3        | 0.94          |
| (1,2493) | 1:887:A:TYR:H    | 1:887:A:TYR:HD1 | 18       | 0.94          |
| (1,973)  | 1:771:A:PHE:HE1  | 1:812:A:PHE:HD2 | 13       | 0.94          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 16       | 0.94          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2493) | 1:887:A:TYR:H    | 1:887:A:TYR:HD1 | 17       | 0.93          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 3        | 0.93          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 5        | 0.93          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 8        | 0.93          |
| (1,1071) | 1:887:A:TYR:HB3  | 1:887:A:TYR:HD1 | 5        | 0.93          |
| (1,1071) | 1:887:A:TYR:HB3  | 1:887:A:TYR:HD1 | 12       | 0.93          |
| (1,1071) | 1:887:A:TYR:HB3  | 1:887:A:TYR:HD1 | 17       | 0.93          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 14       | 0.93          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1 | 4        | 0.93          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1 | 4        | 0.93          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1 | 4        | 0.93          |
| (1,127)  | 1:766:A:LEU:HD11 | 1:771:A:PHE:HD2 | 17       | 0.93          |
| (1,127)  | 1:766:A:LEU:HD12 | 1:771:A:PHE:HD2 | 17       | 0.93          |
| (1,127)  | 1:766:A:LEU:HD13 | 1:771:A:PHE:HD2 | 17       | 0.93          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB2 | 7        | 0.92          |
| (1,2704) | 1:882:A:PHE:HD2  | 1:886:A:LEU:HB3 | 7        | 0.92          |
| (1,1071) | 1:887:A:TYR:HB3  | 1:887:A:TYR:HD1 | 3        | 0.92          |
| (1,1071) | 1:887:A:TYR:HB3  | 1:887:A:TYR:HD1 | 18       | 0.92          |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2 | 13       | 0.92          |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H   | 7        | 0.91          |
| (1,1071) | 1:887:A:TYR:HB3  | 1:887:A:TYR:HD1 | 16       | 0.91          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 16       | 0.91          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 9        | 0.91          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1 | 5        | 0.91          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1 | 5        | 0.91          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1 | 5        | 0.91          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 4        | 0.9           |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2 | 14       | 0.9           |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 13       | 0.9           |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2 | 8        | 0.9           |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 11       | 0.9           |
| (1,2493) | 1:887:A:TYR:H    | 1:887:A:TYR:HD1 | 3        | 0.89          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 10       | 0.89          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 5        | 0.89          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 10       | 0.89          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 12       | 0.89          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 18       | 0.89          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 20       | 0.88          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 3        | 0.88          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 6        | 0.88          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 4        | 0.88          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 5        | 0.88          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 13       | 0.88          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 9        | 0.87          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 10       | 0.87          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 11       | 0.87          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 14       | 0.87          |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2 | 9        | 0.87          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 8        | 0.87          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2 | 2        | 0.87          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 6        | 0.87          |
| (1,818)  | 1:867:A:TYR:HD2  | 1:878:A:ASP:HB2 | 7        | 0.87          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1 | 18       | 0.87          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1 | 18       | 0.87          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1 | 18       | 0.87          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 12       | 0.86          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 15       | 0.86          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 17       | 0.86          |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2 | 15       | 0.86          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 4        | 0.85          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 16       | 0.85          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 18       | 0.85          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 20       | 0.85          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 3        | 0.85          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 5        | 0.85          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 20       | 0.85          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2 | 9        | 0.84          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 1        | 0.84          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 19       | 0.84          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 9        | 0.84          |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2 | 9        | 0.84          |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H   | 16       | 0.83          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 7        | 0.83          |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2 | 12       | 0.83          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 11       | 0.83          |
| (1,2493) | 1:887:A:TYR:H    | 1:887:A:TYR:HD1 | 5        | 0.82          |
| (1,2493) | 1:887:A:TYR:H    | 1:887:A:TYR:HD1 | 12       | 0.82          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 12       | 0.82          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 18       | 0.82          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 2        | 0.82          |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2 | 6        | 0.82          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 1        | 0.82          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 7        | 0.82          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 13       | 0.82          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 15       | 0.82          |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2 | 6        | 0.82          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2 | 2        | 0.82          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2 | 6        | 0.81          |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 8        | 0.81          |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2 | 15       | 0.81          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 14       | 0.81          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2 | 17       | 0.8           |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3 | 17       | 0.8           |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H   | 16       | 0.8           |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H   | 5        | 0.8           |
| (1,1410) | 1:771:A:PHE:H    | 1:771:A:PHE:HD2 | 17       | 0.8           |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2 | 2        | 0.8           |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 2        | 0.8           |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 19       | 0.8           |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2 | 12       | 0.8           |
| (1,2494) | 1:887:A:TYR:H    | 1:887:A:TYR:HE1 | 5        | 0.79          |
| (1,2494) | 1:887:A:TYR:H    | 1:887:A:TYR:HE1 | 12       | 0.79          |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H   | 11       | 0.79          |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H   | 9        | 0.79          |
| (1,937)  | 1:882:A:PHE:HA   | 1:882:A:PHE:HD2 | 6        | 0.79          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2 | 2        | 0.78          |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2 | 13       | 0.78          |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2 | 6        | 0.78          |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2 | 2        | 0.77          |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2 | 16       | 0.76          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2 | 8        | 0.76          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2 | 12       | 0.75          |
| (1,1632) | 1:791:A:GLU:H    | 1:794:A:ARG:HG2 | 11       | 0.75          |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2 | 8        | 0.75          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2 | 15       | 0.75          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1 | 3        | 0.75          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1 | 3        | 0.75          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1 | 3        | 0.75          |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H   | 14       | 0.74          |
| (1,1632) | 1:791:A:GLU:H    | 1:794:A:ARG:HG2 | 3        | 0.74          |
| (1,855)  | 1:867:A:TYR:HE1  | 1:870:A:PRO:HG2 | 14       | 0.74          |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2 | 5        | 0.74          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1 | 17       | 0.74          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1 | 17       | 0.74          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1 | 17       | 0.74          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1 | 2        | 0.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1  | 2        | 0.74          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1  | 2        | 0.74          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1  | 8        | 0.74          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1  | 8        | 0.74          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1  | 8        | 0.74          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1  | 9        | 0.74          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1  | 9        | 0.74          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1  | 9        | 0.74          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2  | 8        | 0.73          |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2  | 3        | 0.73          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1  | 7        | 0.71          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1  | 7        | 0.71          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1  | 7        | 0.71          |
| (1,2478) | 1:882:A:PHE:HD1  | 1:883:A:SER:H    | 17       | 0.7           |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H    | 6        | 0.7           |
| (1,2363) | 1:867:A:TYR:HE1  | 1:871:A:ASP:H    | 9        | 0.7           |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2  | 14       | 0.69          |
| (1,1038) | 1:842:A:TYR:HB2  | 1:867:A:TYR:HD2  | 8        | 0.69          |
| (1,1031) | 1:842:A:TYR:HD1  | 1:867:A:TYR:HD2  | 9        | 0.69          |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 13       | 0.69          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1  | 19       | 0.69          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1  | 19       | 0.69          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1  | 19       | 0.69          |
| (1,1632) | 1:791:A:GLU:H    | 1:794:A:ARG:HG2  | 6        | 0.68          |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2  | 5        | 0.68          |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2  | 9        | 0.68          |
| (1,554)  | 1:829:A:VAL:HG11 | 1:882:A:PHE:HE1  | 10       | 0.68          |
| (1,554)  | 1:829:A:VAL:HG12 | 1:882:A:PHE:HE1  | 10       | 0.68          |
| (1,554)  | 1:829:A:VAL:HG13 | 1:882:A:PHE:HE1  | 10       | 0.68          |
| (1,1038) | 1:842:A:TYR:HB2  | 1:867:A:TYR:HD2  | 6        | 0.67          |
| (1,1038) | 1:842:A:TYR:HB2  | 1:867:A:TYR:HD2  | 12       | 0.67          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2  | 11       | 0.66          |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 15       | 0.66          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 13       | 0.65          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 13       | 0.65          |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H    | 16       | 0.65          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2  | 7        | 0.65          |
| (1,1168) | 1:772:A:LYS:HD3  | 1:784:A:ASN:H    | 11       | 0.65          |
| (1,1038) | 1:842:A:TYR:HB2  | 1:867:A:TYR:HD2  | 15       | 0.65          |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 2        | 0.65          |
| (1,420)  | 1:804:A:LEU:HA   | 1:804:A:LEU:HD21 | 16       | 0.65          |
| (1,420)  | 1:804:A:LEU:HA   | 1:804:A:LEU:HD22 | 16       | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,420)  | 1:804:A:LEU:HA   | 1:804:A:LEU:HD23 | 16       | 0.65          |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H    | 12       | 0.64          |
| (1,1038) | 1:842:A:TYR:HB2  | 1:867:A:TYR:HD2  | 13       | 0.64          |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 9        | 0.64          |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 12       | 0.63          |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2  | 3        | 0.63          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1  | 12       | 0.63          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1  | 12       | 0.63          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1  | 12       | 0.63          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1  | 20       | 0.63          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1  | 20       | 0.63          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1  | 20       | 0.63          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2  | 5        | 0.62          |
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 13       | 0.62          |
| (1,1644) | 1:792:A:PHE:H    | 1:794:A:ARG:HG2  | 15       | 0.62          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2  | 15       | 0.62          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1  | 13       | 0.62          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1  | 13       | 0.62          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1  | 13       | 0.62          |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2  | 16       | 0.61          |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2  | 7        | 0.6           |
| (1,1039) | 1:842:A:TYR:HB3  | 1:867:A:TYR:HD2  | 17       | 0.6           |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2  | 14       | 0.6           |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2  | 15       | 0.59          |
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 17       | 0.59          |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 8        | 0.59          |
| (1,1168) | 1:772:A:LYS:HD3  | 1:784:A:ASN:H    | 20       | 0.58          |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2  | 11       | 0.58          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2  | 3        | 0.58          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2  | 12       | 0.58          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2  | 16       | 0.57          |
| (1,854)  | 1:842:A:TYR:HB2  | 1:867:A:TYR:HE2  | 17       | 0.57          |
| (1,1802) | 1:804:A:LEU:HD11 | 1:806:A:VAL:H    | 16       | 0.56          |
| (1,1802) | 1:804:A:LEU:HD12 | 1:806:A:VAL:H    | 16       | 0.56          |
| (1,1802) | 1:804:A:LEU:HD13 | 1:806:A:VAL:H    | 16       | 0.56          |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 6        | 0.56          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 3        | 0.55          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 3        | 0.55          |
| (1,1038) | 1:842:A:TYR:HB2  | 1:867:A:TYR:HD2  | 5        | 0.55          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2  | 16       | 0.55          |
| (1,2098) | 1:841:A:ASN:HD22 | 1:867:A:TYR:HE2  | 3        | 0.54          |
| (1,1038) | 1:842:A:TYR:HB2  | 1:867:A:TYR:HD2  | 9        | 0.54          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1806) | 1:771:A:PHE:HD1 | 1:807:A:VAL:H    | 11       | 0.53          |
| (1,1038) | 1:842:A:TYR:HB2 | 1:867:A:TYR:HD2  | 2        | 0.53          |
| (1,1806) | 1:771:A:PHE:HD1 | 1:807:A:VAL:H    | 12       | 0.52          |
| (1,1039) | 1:842:A:TYR:HB3 | 1:867:A:TYR:HD2  | 11       | 0.52          |
| (1,856)  | 1:842:A:TYR:HB3 | 1:867:A:TYR:HE2  | 3        | 0.52          |
| (1,356)  | 1:864:A:MET:HE1 | 1:882:A:PHE:HD1  | 15       | 0.52          |
| (1,356)  | 1:864:A:MET:HE2 | 1:882:A:PHE:HD1  | 15       | 0.52          |
| (1,356)  | 1:864:A:MET:HE3 | 1:882:A:PHE:HD1  | 15       | 0.52          |
| (1,1806) | 1:771:A:PHE:HD1 | 1:807:A:VAL:H    | 19       | 0.51          |
| (1,1038) | 1:842:A:TYR:HB2 | 1:867:A:TYR:HD2  | 16       | 0.51          |
| (1,856)  | 1:842:A:TYR:HB3 | 1:867:A:TYR:HE2  | 5        | 0.51          |
| (1,356)  | 1:864:A:MET:HE1 | 1:882:A:PHE:HD1  | 11       | 0.51          |
| (1,356)  | 1:864:A:MET:HE2 | 1:882:A:PHE:HD1  | 11       | 0.51          |
| (1,356)  | 1:864:A:MET:HE3 | 1:882:A:PHE:HD1  | 11       | 0.51          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD2  | 17       | 0.5           |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD3  | 17       | 0.5           |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD2  | 17       | 0.5           |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD3  | 17       | 0.5           |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD11 | 3        | 0.49          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD12 | 3        | 0.49          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD13 | 3        | 0.49          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD11 | 11       | 0.49          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD12 | 11       | 0.49          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD13 | 11       | 0.49          |
| (1,1806) | 1:771:A:PHE:HD1 | 1:807:A:VAL:H    | 16       | 0.49          |
| (1,854)  | 1:842:A:TYR:HB2 | 1:867:A:TYR:HE2  | 7        | 0.49          |
| (1,2694) | 1:867:A:TYR:HE1 | 1:871:A:ASP:HB2  | 8        | 0.48          |
| (1,2694) | 1:867:A:TYR:HE1 | 1:871:A:ASP:HB3  | 8        | 0.48          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG2  | 1        | 0.48          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG3  | 1        | 0.48          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG2  | 1        | 0.48          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG3  | 1        | 0.48          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD11 | 5        | 0.48          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD12 | 5        | 0.48          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD13 | 5        | 0.48          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD11 | 7        | 0.48          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD12 | 7        | 0.48          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD13 | 7        | 0.48          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD11 | 13       | 0.48          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD12 | 13       | 0.48          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD13 | 13       | 0.48          |
| (1,1806) | 1:771:A:PHE:HD1 | 1:807:A:VAL:H    | 2        | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 7        | 0.48          |
| (1,1038) | 1:842:A:TYR:HB2  | 1:867:A:TYR:HD2  | 14       | 0.48          |
| (1,825)  | 1:882:A:PHE:HD1  | 1:883:A:SER:HA   | 1        | 0.48          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 14       | 0.47          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 14       | 0.47          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 5        | 0.47          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 5        | 0.47          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 5        | 0.47          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 5        | 0.47          |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG11 | 10       | 0.47          |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG12 | 10       | 0.47          |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG13 | 10       | 0.47          |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG21 | 10       | 0.47          |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG22 | 10       | 0.47          |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG23 | 10       | 0.47          |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H    | 3        | 0.47          |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H    | 17       | 0.47          |
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 8        | 0.47          |
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 20       | 0.47          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 3        | 0.47          |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 16       | 0.47          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 20       | 0.46          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 20       | 0.46          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 20       | 0.46          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 20       | 0.46          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 6        | 0.46          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 6        | 0.46          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD2  | 6        | 0.46          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD3  | 6        | 0.46          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 14       | 0.46          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 14       | 0.46          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 14       | 0.46          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB1  | 8        | 0.46          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB2  | 8        | 0.46          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB3  | 8        | 0.46          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 17       | 0.44          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 17       | 0.44          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 17       | 0.44          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 17       | 0.44          |
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 1        | 0.44          |
| (1,1038) | 1:842:A:TYR:HB2  | 1:867:A:TYR:HD2  | 3        | 0.44          |
| (1,1034) | 1:867:A:TYR:H    | 1:867:A:TYR:HD1  | 8        | 0.44          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1034) | 1:867:A:TYR:H   | 1:867:A:TYR:HD1  | 9        | 0.44          |
| (1,2716) | 1:887:A:TYR:HE2 | 1:888:A:GLY:HA2  | 3        | 0.43          |
| (1,2716) | 1:887:A:TYR:HE2 | 1:888:A:GLY:HA3  | 3        | 0.43          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG2  | 9        | 0.43          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG3  | 9        | 0.43          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG2  | 9        | 0.43          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG3  | 9        | 0.43          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG2  | 13       | 0.43          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG3  | 13       | 0.43          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG2  | 13       | 0.43          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG3  | 13       | 0.43          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD2  | 5        | 0.43          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD3  | 5        | 0.43          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD2  | 5        | 0.43          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD3  | 5        | 0.43          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE21 | 1        | 0.43          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE22 | 1        | 0.43          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE21 | 1        | 0.43          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE22 | 1        | 0.43          |
| (1,2362) | 1:867:A:TYR:HE1 | 1:869:A:GLY:H    | 11       | 0.43          |
| (1,1031) | 1:842:A:TYR:HD1 | 1:867:A:TYR:HD2  | 2        | 0.43          |
| (1,852)  | 1:842:A:TYR:HD1 | 1:867:A:TYR:HE2  | 14       | 0.43          |
| (1,825)  | 1:882:A:PHE:HD1 | 1:883:A:SER:HA   | 7        | 0.43          |
| (1,825)  | 1:882:A:PHE:HD1 | 1:883:A:SER:HA   | 9        | 0.43          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD11 | 16       | 0.42          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD12 | 16       | 0.42          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD13 | 16       | 0.42          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD21 | 16       | 0.42          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD22 | 16       | 0.42          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD23 | 16       | 0.42          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD11 | 16       | 0.42          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD12 | 16       | 0.42          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD13 | 16       | 0.42          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD21 | 16       | 0.42          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD22 | 16       | 0.42          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD23 | 16       | 0.42          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG2  | 4        | 0.42          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG3  | 4        | 0.42          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG2  | 4        | 0.42          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG3  | 4        | 0.42          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD2  | 13       | 0.42          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD3  | 13       | 0.42          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD2  | 13       | 0.42          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD3  | 13       | 0.42          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD2  | 18       | 0.42          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD3  | 18       | 0.42          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD2  | 18       | 0.42          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD3  | 18       | 0.42          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD2  | 20       | 0.42          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD3  | 20       | 0.42          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD2  | 20       | 0.42          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD3  | 20       | 0.42          |
| (1,2623) | 1:826:A:ALA:HA  | 1:829:A:VAL:HG11 | 20       | 0.42          |
| (1,2623) | 1:826:A:ALA:HA  | 1:829:A:VAL:HG12 | 20       | 0.42          |
| (1,2623) | 1:826:A:ALA:HA  | 1:829:A:VAL:HG13 | 20       | 0.42          |
| (1,2623) | 1:826:A:ALA:HA  | 1:829:A:VAL:HG21 | 20       | 0.42          |
| (1,2623) | 1:826:A:ALA:HA  | 1:829:A:VAL:HG22 | 20       | 0.42          |
| (1,2623) | 1:826:A:ALA:HA  | 1:829:A:VAL:HG23 | 20       | 0.42          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD11 | 18       | 0.42          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD12 | 18       | 0.42          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD13 | 18       | 0.42          |
| (1,1038) | 1:842:A:TYR:HB2 | 1:867:A:TYR:HD2  | 17       | 0.42          |
| (1,1034) | 1:867:A:TYR:H   | 1:867:A:TYR:HD1  | 13       | 0.42          |
| (1,1034) | 1:867:A:TYR:H   | 1:867:A:TYR:HD1  | 14       | 0.42          |
| (1,825)  | 1:882:A:PHE:HD1 | 1:883:A:SER:HA   | 6        | 0.42          |
| (1,356)  | 1:864:A:MET:HE1 | 1:882:A:PHE:HD1  | 6        | 0.42          |
| (1,356)  | 1:864:A:MET:HE2 | 1:882:A:PHE:HD1  | 6        | 0.42          |
| (1,356)  | 1:864:A:MET:HE3 | 1:882:A:PHE:HD1  | 6        | 0.42          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE21 | 5        | 0.41          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE22 | 5        | 0.41          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE21 | 5        | 0.41          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE22 | 5        | 0.41          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE21 | 13       | 0.41          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE22 | 13       | 0.41          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE21 | 13       | 0.41          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE22 | 13       | 0.41          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE21 | 20       | 0.41          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE22 | 20       | 0.41          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE21 | 20       | 0.41          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE22 | 20       | 0.41          |
| (1,2362) | 1:867:A:TYR:HE1 | 1:869:A:GLY:H    | 5        | 0.41          |
| (1,1168) | 1:772:A:LYS:HD3 | 1:784:A:ASN:H    | 8        | 0.41          |
| (1,856)  | 1:842:A:TYR:HB3 | 1:867:A:TYR:HE2  | 14       | 0.41          |
| (1,852)  | 1:842:A:TYR:HD1 | 1:867:A:TYR:HE2  | 6        | 0.41          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,825)  | 1:882:A:PHE:HD1 | 1:883:A:SER:HA   | 2        | 0.41          |
| (1,825)  | 1:882:A:PHE:HD1 | 1:883:A:SER:HA   | 14       | 0.41          |
| (1,825)  | 1:882:A:PHE:HD1 | 1:883:A:SER:HA   | 19       | 0.41          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG2  | 6        | 0.4           |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG3  | 6        | 0.4           |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG2  | 6        | 0.4           |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG3  | 6        | 0.4           |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD2  | 11       | 0.4           |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD3  | 11       | 0.4           |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD2  | 11       | 0.4           |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD3  | 11       | 0.4           |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE21 | 11       | 0.4           |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE22 | 11       | 0.4           |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE21 | 11       | 0.4           |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE22 | 11       | 0.4           |
| (1,2362) | 1:867:A:TYR:HE1 | 1:869:A:GLY:H    | 7        | 0.4           |
| (1,1806) | 1:771:A:PHE:HD1 | 1:807:A:VAL:H    | 5        | 0.4           |
| (1,1034) | 1:867:A:TYR:H   | 1:867:A:TYR:HD1  | 11       | 0.4           |
| (1,1031) | 1:842:A:TYR:HD1 | 1:867:A:TYR:HD2  | 15       | 0.4           |
| (1,2694) | 1:867:A:TYR:HE1 | 1:871:A:ASP:HB2  | 11       | 0.39          |
| (1,2694) | 1:867:A:TYR:HE1 | 1:871:A:ASP:HB3  | 11       | 0.39          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG2  | 14       | 0.39          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG3  | 14       | 0.39          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG2  | 14       | 0.39          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG3  | 14       | 0.39          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE21 | 4        | 0.39          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE22 | 4        | 0.39          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE21 | 4        | 0.39          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE22 | 4        | 0.39          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE21 | 9        | 0.39          |
| (1,2537) | 1:745:A:GLN:HG2 | 1:745:A:GLN:HE22 | 9        | 0.39          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE21 | 9        | 0.39          |
| (1,2537) | 1:745:A:GLN:HG3 | 1:745:A:GLN:HE22 | 9        | 0.39          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD11 | 1        | 0.39          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD12 | 1        | 0.39          |
| (1,2088) | 1:840:A:LYS:H   | 1:843:A:ILE:HD13 | 1        | 0.39          |
| (1,1034) | 1:867:A:TYR:H   | 1:867:A:TYR:HD1  | 3        | 0.39          |
| (1,1034) | 1:867:A:TYR:H   | 1:867:A:TYR:HD1  | 12       | 0.39          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG2  | 7        | 0.38          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG3  | 7        | 0.38          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG2  | 7        | 0.38          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG3  | 7        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 1        | 0.38          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 1        | 0.38          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD2  | 1        | 0.38          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD3  | 1        | 0.38          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 6        | 0.38          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 6        | 0.38          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 6        | 0.38          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 6        | 0.38          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 7        | 0.38          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 7        | 0.38          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 7        | 0.38          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 7        | 0.38          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 14       | 0.38          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 14       | 0.38          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 14       | 0.38          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 14       | 0.38          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 18       | 0.38          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 18       | 0.38          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 18       | 0.38          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 18       | 0.38          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 4        | 0.38          |
| (1,1034) | 1:867:A:TYR:H    | 1:867:A:TYR:HD1  | 5        | 0.38          |
| (1,1034) | 1:867:A:TYR:H    | 1:867:A:TYR:HD1  | 7        | 0.38          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 10       | 0.37          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 10       | 0.37          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 10       | 0.37          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 10       | 0.37          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 13       | 0.37          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 13       | 0.37          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 13       | 0.37          |
| (1,2362) | 1:867:A:TYR:HE1  | 1:869:A:GLY:H    | 14       | 0.37          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 16       | 0.37          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 17       | 0.36          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 17       | 0.36          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 17       | 0.36          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 17       | 0.36          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 18       | 0.36          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 18       | 0.36          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 18       | 0.36          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 18       | 0.36          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 3        | 0.36          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 3        | 0.36          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD2  | 3        | 0.36          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD3  | 3        | 0.36          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD2  | 7        | 0.36          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD3  | 7        | 0.36          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD2  | 7        | 0.36          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD3  | 7        | 0.36          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD2  | 9        | 0.36          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD3  | 9        | 0.36          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD2  | 9        | 0.36          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD3  | 9        | 0.36          |
| (1,2072) | 1:838:A:GLY:H   | 1:839:A:ASP:HA   | 17       | 0.36          |
| (1,1806) | 1:771:A:PHE:HD1 | 1:807:A:VAL:H    | 9        | 0.36          |
| (1,1806) | 1:771:A:PHE:HD1 | 1:807:A:VAL:H    | 14       | 0.36          |
| (1,1806) | 1:771:A:PHE:HD1 | 1:807:A:VAL:H    | 15       | 0.36          |
| (1,1038) | 1:842:A:TYR:HB2 | 1:867:A:TYR:HD2  | 11       | 0.36          |
| (1,950)  | 1:775:A:LEU:HB2 | 1:780:A:TYR:HD1  | 11       | 0.36          |
| (1,804)  | 1:845:A:MET:HE1 | 1:877:A:LEU:HD21 | 20       | 0.36          |
| (1,804)  | 1:845:A:MET:HE1 | 1:877:A:LEU:HD22 | 20       | 0.36          |
| (1,804)  | 1:845:A:MET:HE1 | 1:877:A:LEU:HD23 | 20       | 0.36          |
| (1,804)  | 1:845:A:MET:HE2 | 1:877:A:LEU:HD21 | 20       | 0.36          |
| (1,804)  | 1:845:A:MET:HE2 | 1:877:A:LEU:HD22 | 20       | 0.36          |
| (1,804)  | 1:845:A:MET:HE2 | 1:877:A:LEU:HD23 | 20       | 0.36          |
| (1,804)  | 1:845:A:MET:HE3 | 1:877:A:LEU:HD21 | 20       | 0.36          |
| (1,804)  | 1:845:A:MET:HE3 | 1:877:A:LEU:HD22 | 20       | 0.36          |
| (1,804)  | 1:845:A:MET:HE3 | 1:877:A:LEU:HD23 | 20       | 0.36          |
| (1,2716) | 1:887:A:TYR:HE2 | 1:888:A:GLY:HA2  | 5        | 0.35          |
| (1,2716) | 1:887:A:TYR:HE2 | 1:888:A:GLY:HA3  | 5        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD11 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD12 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD13 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD21 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD22 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD23 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD11 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD12 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD13 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD21 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD22 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD23 | 3        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD11 | 6        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD12 | 6        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD13 | 6        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 6        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 6        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 6        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 6        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 6        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 6        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 6        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 6        | 0.35          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 6        | 0.35          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 10       | 0.35          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 10       | 0.35          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 10       | 0.35          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 10       | 0.35          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 16       | 0.35          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 16       | 0.35          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD2  | 16       | 0.35          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD3  | 16       | 0.35          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 3        | 0.35          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 3        | 0.35          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 3        | 0.35          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 3        | 0.35          |
| (1,2493) | 1:887:A:TYR:H    | 1:887:A:TYR:HD1  | 16       | 0.35          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 1        | 0.35          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 1        | 0.35          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 1        | 0.35          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 9        | 0.35          |
| (1,1167) | 1:743:A:ILE:HG13 | 1:748:A:MET:H    | 7        | 0.35          |
| (1,1034) | 1:867:A:TYR:H    | 1:867:A:TYR:HD1  | 2        | 0.35          |
| (1,1034) | 1:867:A:TYR:H    | 1:867:A:TYR:HD1  | 15       | 0.35          |
| (1,1031) | 1:842:A:TYR:HD1  | 1:867:A:TYR:HD2  | 12       | 0.35          |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 17       | 0.35          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB1  | 14       | 0.35          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB2  | 14       | 0.35          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB3  | 14       | 0.35          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 7        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 7        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 7        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 7        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 7        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 7        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 7        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 7        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 7        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 7        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 7        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 7        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 18       | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 18       | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 18       | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 18       | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 18       | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 18       | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 18       | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 18       | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 18       | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 18       | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 18       | 0.34          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 18       | 0.34          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 11       | 0.34          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 11       | 0.34          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 11       | 0.34          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 11       | 0.34          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 15       | 0.34          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 15       | 0.34          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 15       | 0.34          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 15       | 0.34          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 4        | 0.34          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 4        | 0.34          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD2  | 4        | 0.34          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD3  | 4        | 0.34          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 9        | 0.34          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 9        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 9        | 0.34          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 9        | 0.34          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 9        | 0.34          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 9        | 0.34          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 8        | 0.34          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 8        | 0.34          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 8        | 0.34          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 8        | 0.34          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 17       | 0.34          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 17       | 0.34          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 17       | 0.34          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 17       | 0.34          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 17       | 0.34          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 17       | 0.34          |
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 6        | 0.34          |
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 10       | 0.34          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 15       | 0.34          |
| (1,1038) | 1:842:A:TYR:HB2  | 1:867:A:TYR:HD2  | 7        | 0.34          |
| (1,1034) | 1:867:A:TYR:H    | 1:867:A:TYR:HD1  | 6        | 0.34          |
| (1,1034) | 1:867:A:TYR:H    | 1:867:A:TYR:HD1  | 17       | 0.34          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 13       | 0.34          |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 7        | 0.34          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2  | 5        | 0.34          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2  | 9        | 0.34          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 1        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 4        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 4        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 4        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 4        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 4        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 4        | 0.33          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD11 | 4        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD12 | 4        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD13 | 4        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD21 | 4        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD22 | 4        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD23 | 4        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD11 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD12 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD13 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD21 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD22 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD23 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD11 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD12 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD13 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD21 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD22 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD23 | 5        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD11 | 8        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD12 | 8        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD13 | 8        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD21 | 8        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD22 | 8        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2 | 1:886:A:LEU:HD23 | 8        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD11 | 8        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD12 | 8        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD13 | 8        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD21 | 8        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD22 | 8        | 0.33          |
| (1,2711) | 1:886:A:LEU:HB3 | 1:886:A:LEU:HD23 | 8        | 0.33          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG2  | 3        | 0.33          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG3  | 3        | 0.33          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG2  | 3        | 0.33          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG3  | 3        | 0.33          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG2  | 16       | 0.33          |
| (1,2679) | 1:850:A:ARG:HG2 | 1:851:A:GLU:HG3  | 16       | 0.33          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG2  | 16       | 0.33          |
| (1,2679) | 1:850:A:ARG:HG3 | 1:851:A:GLU:HG3  | 16       | 0.33          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD2  | 2        | 0.33          |
| (1,2672) | 1:849:A:ARG:HB2 | 1:849:A:ARG:HD3  | 2        | 0.33          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD2  | 2        | 0.33          |
| (1,2672) | 1:849:A:ARG:HB3 | 1:849:A:ARG:HD3  | 2        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 14       | 0.33          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 14       | 0.33          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD2  | 14       | 0.33          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD3  | 14       | 0.33          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 13       | 0.33          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 13       | 0.33          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 13       | 0.33          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 13       | 0.33          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 13       | 0.33          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 13       | 0.33          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 15       | 0.33          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 15       | 0.33          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 15       | 0.33          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 15       | 0.33          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 9        | 0.33          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 9        | 0.33          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 9        | 0.33          |
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 4        | 0.33          |
| (1,1671) | 1:794:A:ARG:HG2  | 1:795:A:ILE:H    | 3        | 0.33          |
| (1,1671) | 1:794:A:ARG:HG2  | 1:795:A:ILE:H    | 11       | 0.33          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 6        | 0.33          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 5        | 0.33          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 6        | 0.33          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 14       | 0.33          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2  | 8        | 0.33          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2  | 13       | 0.33          |
| (1,825)  | 1:882:A:PHE:HD1  | 1:883:A:SER:HA   | 11       | 0.33          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 11       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 14       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 14       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 14       | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 14       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 14       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 14       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 14       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 14       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 14       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 14       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 14       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 14       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 15       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 15       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 15       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 15       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 15       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 15       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 15       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 15       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 15       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 15       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 15       | 0.32          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 15       | 0.32          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 19       | 0.32          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 19       | 0.32          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD2  | 19       | 0.32          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD3  | 19       | 0.32          |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 10       | 0.32          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 10       | 0.32          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 10       | 0.32          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 10       | 0.32          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 10       | 0.32          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 10       | 0.32          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 18       | 0.32          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 18       | 0.32          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 18       | 0.32          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 18       | 0.32          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 18       | 0.32          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 18       | 0.32          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 4        | 0.32          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 4        | 0.32          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 4        | 0.32          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 6        | 0.32          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 6        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 6        | 0.32          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 13       | 0.32          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 13       | 0.32          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 13       | 0.32          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 15       | 0.32          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 15       | 0.32          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 15       | 0.32          |
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 18       | 0.32          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 1        | 0.32          |
| (1,1031) | 1:842:A:TYR:HD1  | 1:867:A:TYR:HD2  | 16       | 0.32          |
| (1,856)  | 1:842:A:TYR:HB3  | 1:867:A:TYR:HE2  | 11       | 0.32          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2  | 6        | 0.32          |
| (1,825)  | 1:882:A:PHE:HD1  | 1:883:A:SER:HA   | 3        | 0.32          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 17       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 20       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 20       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 20       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 20       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 20       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 20       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 20       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 20       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 20       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 20       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 20       | 0.31          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 20       | 0.31          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 8        | 0.31          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 8        | 0.31          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 8        | 0.31          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 8        | 0.31          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 8        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 8        | 0.31          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD2  | 8        | 0.31          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD3  | 8        | 0.31          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 10       | 0.31          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 10       | 0.31          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD2  | 10       | 0.31          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD3  | 10       | 0.31          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 15       | 0.31          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 15       | 0.31          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD2  | 15       | 0.31          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD3  | 15       | 0.31          |
| (1,1806) | 1:771:A:PHE:HD1  | 1:807:A:VAL:H    | 3        | 0.31          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 2        | 0.31          |
| (1,1122) | 1:745:A:GLN:HB2  | 1:745:A:GLN:HE22 | 20       | 0.31          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 1        | 0.31          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 6        | 0.31          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 20       | 0.31          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2  | 12       | 0.31          |
| (1,825)  | 1:882:A:PHE:HD1  | 1:883:A:SER:HA   | 8        | 0.31          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 11       | 0.31          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 11       | 0.31          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 11       | 0.31          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 11       | 0.31          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 11       | 0.31          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 11       | 0.31          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 11       | 0.31          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 11       | 0.31          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 11       | 0.31          |
| (1,2716) | 1:887:A:TYR:HE2  | 1:888:A:GLY:HA2  | 12       | 0.3           |
| (1,2716) | 1:887:A:TYR:HE2  | 1:888:A:GLY:HA3  | 12       | 0.3           |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 7        | 0.3           |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 7        | 0.3           |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 2        | 0.3           |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 2        | 0.3           |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 2        | 0.3           |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 2        | 0.3           |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 16       | 0.3           |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 16       | 0.3           |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 16       | 0.3           |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 16       | 0.3           |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 20       | 0.3           |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 20       | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 20       | 0.3           |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 16       | 0.3           |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 16       | 0.3           |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 16       | 0.3           |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 10       | 0.3           |
| (1,1034) | 1:867:A:TYR:H    | 1:867:A:TYR:HD1  | 16       | 0.3           |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 13       | 0.3           |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 13       | 0.3           |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 13       | 0.3           |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 13       | 0.3           |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 13       | 0.3           |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 13       | 0.3           |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 13       | 0.3           |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 13       | 0.3           |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 13       | 0.3           |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 17       | 0.3           |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 17       | 0.3           |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 17       | 0.3           |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 17       | 0.3           |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 17       | 0.3           |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 17       | 0.3           |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 17       | 0.3           |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 17       | 0.3           |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 17       | 0.3           |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 12       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 19       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 19       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 19       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 19       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 19       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 19       | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 19       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 19       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 19       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 19       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 19       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 19       | 0.29          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 12       | 0.29          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 12       | 0.29          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 12       | 0.29          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 12       | 0.29          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 12       | 0.29          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 12       | 0.29          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 7        | 0.29          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 7        | 0.29          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 7        | 0.29          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 7        | 0.29          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 7        | 0.29          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 7        | 0.29          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 12       | 0.29          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 12       | 0.29          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 12       | 0.29          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 12       | 0.29          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 9        | 0.29          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 13       | 0.29          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 7        | 0.29          |
| (1,825)  | 1:882:A:PHE:HD1  | 1:883:A:SER:HA   | 5        | 0.29          |
| (1,825)  | 1:882:A:PHE:HD1  | 1:883:A:SER:HA   | 13       | 0.29          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1  | 17       | 0.29          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1  | 17       | 0.29          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1  | 17       | 0.29          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 10       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 10       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 10       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 10       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 10       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 10       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 10       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 10       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 10       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 10       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 10       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 10       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 13       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 13       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 13       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 13       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 13       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 13       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 13       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 13       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 13       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 13       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 13       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 13       | 0.28          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD2  | 12       | 0.28          |
| (1,2672) | 1:849:A:ARG:HB2  | 1:849:A:ARG:HD3  | 12       | 0.28          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD2  | 12       | 0.28          |
| (1,2672) | 1:849:A:ARG:HB3  | 1:849:A:ARG:HD3  | 12       | 0.28          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 19       | 0.28          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 19       | 0.28          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 19       | 0.28          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 19       | 0.28          |
| (1,2494) | 1:887:A:TYR:H    | 1:887:A:TYR:HE1  | 16       | 0.28          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 17       | 0.28          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 17       | 0.28          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 17       | 0.28          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 12       | 0.28          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2  | 16       | 0.28          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 14       | 0.28          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 14       | 0.28          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 14       | 0.28          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 14       | 0.28          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 14       | 0.28          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 14       | 0.28          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 14       | 0.28          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 14       | 0.28          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 14       | 0.28          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD11 | 2        | 0.27          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD12 | 2        | 0.27          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD13 | 2        | 0.27          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD21 | 2        | 0.27          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD22 | 2        | 0.27          |
| (1,2711) | 1:886:A:LEU:HB2  | 1:886:A:LEU:HD23 | 2        | 0.27          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD11 | 2        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD12 | 2        | 0.27          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD13 | 2        | 0.27          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD21 | 2        | 0.27          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD22 | 2        | 0.27          |
| (1,2711) | 1:886:A:LEU:HB3  | 1:886:A:LEU:HD23 | 2        | 0.27          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 3        | 0.27          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 3        | 0.27          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 3        | 0.27          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 3        | 0.27          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 3        | 0.27          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 3        | 0.27          |
| (1,2609) | 1:818:A:ARG:HB2  | 1:819:A:GLU:H    | 10       | 0.27          |
| (1,2609) | 1:818:A:ARG:HB3  | 1:819:A:GLU:H    | 10       | 0.27          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE21 | 2        | 0.27          |
| (1,2537) | 1:745:A:GLN:HG2  | 1:745:A:GLN:HE22 | 2        | 0.27          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE21 | 2        | 0.27          |
| (1,2537) | 1:745:A:GLN:HG3  | 1:745:A:GLN:HE22 | 2        | 0.27          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 13       | 0.27          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 13       | 0.27          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 13       | 0.27          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 17       | 0.27          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 17       | 0.27          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 17       | 0.27          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 7        | 0.27          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 11       | 0.27          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 20       | 0.27          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 11       | 0.27          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 5        | 0.27          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG2  | 19       | 0.26          |
| (1,2679) | 1:850:A:ARG:HG2  | 1:851:A:GLU:HG3  | 19       | 0.26          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG2  | 19       | 0.26          |
| (1,2679) | 1:850:A:ARG:HG3  | 1:851:A:GLU:HG3  | 19       | 0.26          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 17       | 0.26          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 17       | 0.26          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 17       | 0.26          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 17       | 0.26          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 17       | 0.26          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 17       | 0.26          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 6        | 0.26          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 6        | 0.26          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 6        | 0.26          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 20       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 20       | 0.26          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 20       | 0.26          |
| (1,1971) | 1:820:A:THR:HG21 | 1:821:A:ALA:H    | 9        | 0.26          |
| (1,1971) | 1:820:A:THR:HG22 | 1:821:A:ALA:H    | 9        | 0.26          |
| (1,1971) | 1:820:A:THR:HG23 | 1:821:A:ALA:H    | 9        | 0.26          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 1        | 0.26          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 1        | 0.26          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 1        | 0.26          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 7        | 0.26          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 18       | 0.26          |
| (1,1031) | 1:842:A:TYR:HD1  | 1:867:A:TYR:HD2  | 3        | 0.26          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 3        | 0.26          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2  | 7        | 0.26          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 4        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 4        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 4        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 4        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 4        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 4        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 6        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 6        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 6        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 6        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 6        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 6        | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 11       | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 11       | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 11       | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 11       | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 11       | 0.25          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 11       | 0.25          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 11       | 0.25          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 11       | 0.25          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 11       | 0.25          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 5        | 0.25          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 5        | 0.25          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 5        | 0.25          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 9        | 0.25          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 9        | 0.25          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 9        | 0.25          |
| (1,1554) | 1:772:A:LYS:HD2  | 1:783:A:GLY:H    | 13       | 0.25          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 5        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 8        | 0.25          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 9        | 0.25          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 12       | 0.25          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 12       | 0.25          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 12       | 0.25          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 12       | 0.25          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 12       | 0.25          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 12       | 0.25          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 12       | 0.25          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 12       | 0.25          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 12       | 0.25          |
| (1,296)  | 1:772:A:LYS:HD2  | 1:782:A:ILE:HG21 | 8        | 0.25          |
| (1,296)  | 1:772:A:LYS:HD2  | 1:782:A:ILE:HG22 | 8        | 0.25          |
| (1,296)  | 1:772:A:LYS:HD2  | 1:782:A:ILE:HG23 | 8        | 0.25          |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 13       | 0.24          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 13       | 0.24          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 13       | 0.24          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 13       | 0.24          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 13       | 0.24          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 13       | 0.24          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 10       | 0.24          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 10       | 0.24          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 10       | 0.24          |
| (1,2453) | 1:865:A:ALA:HB1  | 1:880:A:MET:H    | 13       | 0.24          |
| (1,2453) | 1:865:A:ALA:HB2  | 1:880:A:MET:H    | 13       | 0.24          |
| (1,2453) | 1:865:A:ALA:HB3  | 1:880:A:MET:H    | 13       | 0.24          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 2        | 0.24          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 2        | 0.24          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 2        | 0.24          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 19       | 0.24          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 19       | 0.24          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 19       | 0.24          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 13       | 0.24          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 13       | 0.24          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 13       | 0.24          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 3        | 0.24          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 3        | 0.24          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 3        | 0.24          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 6        | 0.24          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 6        | 0.24          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 6        | 0.24          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 20       | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 20       | 0.24          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 20       | 0.24          |
| (1,1168) | 1:772:A:LYS:HD3  | 1:784:A:ASN:H    | 18       | 0.24          |
| (1,1031) | 1:842:A:TYR:HD1  | 1:867:A:TYR:HD2  | 14       | 0.24          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2  | 7        | 0.24          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 6        | 0.24          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 6        | 0.24          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 6        | 0.24          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 6        | 0.24          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 6        | 0.24          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 6        | 0.24          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 6        | 0.24          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 6        | 0.24          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 6        | 0.24          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 9        | 0.24          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 9        | 0.24          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 9        | 0.24          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 9        | 0.24          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 9        | 0.24          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 9        | 0.24          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 9        | 0.24          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 9        | 0.24          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 9        | 0.24          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB1  | 18       | 0.24          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB2  | 18       | 0.24          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB3  | 18       | 0.24          |
| (1,2585) | 1:793:A:ALA:HB1  | 1:794:A:ARG:HD2  | 17       | 0.23          |
| (1,2585) | 1:793:A:ALA:HB1  | 1:794:A:ARG:HD3  | 17       | 0.23          |
| (1,2585) | 1:793:A:ALA:HB2  | 1:794:A:ARG:HD2  | 17       | 0.23          |
| (1,2585) | 1:793:A:ALA:HB2  | 1:794:A:ARG:HD3  | 17       | 0.23          |
| (1,2585) | 1:793:A:ALA:HB3  | 1:794:A:ARG:HD2  | 17       | 0.23          |
| (1,2585) | 1:793:A:ALA:HB3  | 1:794:A:ARG:HD3  | 17       | 0.23          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 11       | 0.23          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 11       | 0.23          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 11       | 0.23          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 18       | 0.23          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 18       | 0.23          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 18       | 0.23          |
| (1,1644) | 1:792:A:PHE:H    | 1:794:A:ARG:HG2  | 13       | 0.23          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 1        | 0.23          |
| (1,1486) | 1:775:A:LEU:HD11 | 1:776:A:ILE:H    | 13       | 0.23          |
| (1,1486) | 1:775:A:LEU:HD12 | 1:776:A:ILE:H    | 13       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1486) | 1:775:A:LEU:HD13 | 1:776:A:ILE:H    | 13       | 0.23          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 17       | 0.23          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 19       | 0.23          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 20       | 0.23          |
| (1,1167) | 1:743:A:ILE:HG13 | 1:748:A:MET:H    | 11       | 0.23          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 8        | 0.23          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2  | 14       | 0.23          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 1        | 0.23          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 1        | 0.23          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 1        | 0.23          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 2        | 0.22          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 2        | 0.22          |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 9        | 0.22          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 9        | 0.22          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 9        | 0.22          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 9        | 0.22          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 9        | 0.22          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 9        | 0.22          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 12       | 0.22          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 12       | 0.22          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 12       | 0.22          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 12       | 0.22          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 12       | 0.22          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 12       | 0.22          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 8        | 0.22          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 8        | 0.22          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 8        | 0.22          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 7        | 0.22          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 7        | 0.22          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 7        | 0.22          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 4        | 0.22          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 4        | 0.22          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 4        | 0.22          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 17       | 0.22          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 17       | 0.22          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 17       | 0.22          |
| (1,1856) | 1:808:A:THR:HG21 | 1:810:A:GLN:H    | 1        | 0.22          |
| (1,1856) | 1:808:A:THR:HG22 | 1:810:A:GLN:H    | 1        | 0.22          |
| (1,1856) | 1:808:A:THR:HG23 | 1:810:A:GLN:H    | 1        | 0.22          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 10       | 0.22          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 10       | 0.22          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 10       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 4        | 0.22          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 10       | 0.22          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 17       | 0.22          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2  | 17       | 0.22          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2  | 3        | 0.22          |
| (1,847)  | 1:867:A:TYR:HE1  | 1:869:A:GLY:HA2  | 5        | 0.22          |
| (1,369)  | 1:795:A:ILE:HG21 | 1:798:A:ILE:HD11 | 14       | 0.22          |
| (1,369)  | 1:795:A:ILE:HG21 | 1:798:A:ILE:HD12 | 14       | 0.22          |
| (1,369)  | 1:795:A:ILE:HG21 | 1:798:A:ILE:HD13 | 14       | 0.22          |
| (1,369)  | 1:795:A:ILE:HG22 | 1:798:A:ILE:HD11 | 14       | 0.22          |
| (1,369)  | 1:795:A:ILE:HG22 | 1:798:A:ILE:HD12 | 14       | 0.22          |
| (1,369)  | 1:795:A:ILE:HG22 | 1:798:A:ILE:HD13 | 14       | 0.22          |
| (1,369)  | 1:795:A:ILE:HG23 | 1:798:A:ILE:HD11 | 14       | 0.22          |
| (1,369)  | 1:795:A:ILE:HG23 | 1:798:A:ILE:HD12 | 14       | 0.22          |
| (1,369)  | 1:795:A:ILE:HG23 | 1:798:A:ILE:HD13 | 14       | 0.22          |
| (1,356)  | 1:864:A:MET:HE1  | 1:882:A:PHE:HD1  | 16       | 0.22          |
| (1,356)  | 1:864:A:MET:HE2  | 1:882:A:PHE:HD1  | 16       | 0.22          |
| (1,356)  | 1:864:A:MET:HE3  | 1:882:A:PHE:HD1  | 16       | 0.22          |
| (1,2716) | 1:887:A:TYR:HE2  | 1:888:A:GLY:HA2  | 17       | 0.21          |
| (1,2716) | 1:887:A:TYR:HE2  | 1:888:A:GLY:HA3  | 17       | 0.21          |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 14       | 0.21          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 14       | 0.21          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 14       | 0.21          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 14       | 0.21          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 14       | 0.21          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 14       | 0.21          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 1        | 0.21          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 1        | 0.21          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 1        | 0.21          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 7        | 0.21          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 7        | 0.21          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 7        | 0.21          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 9        | 0.21          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 9        | 0.21          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 9        | 0.21          |
| (1,1971) | 1:820:A:THR:HG21 | 1:821:A:ALA:H    | 15       | 0.21          |
| (1,1971) | 1:820:A:THR:HG22 | 1:821:A:ALA:H    | 15       | 0.21          |
| (1,1971) | 1:820:A:THR:HG23 | 1:821:A:ALA:H    | 15       | 0.21          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 17       | 0.21          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 17       | 0.21          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 17       | 0.21          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 8        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 8        | 0.21          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 8        | 0.21          |
| (1,1595) | 1:782:A:ILE:HG21 | 1:788:A:GLY:H    | 11       | 0.21          |
| (1,1595) | 1:782:A:ILE:HG22 | 1:788:A:GLY:H    | 11       | 0.21          |
| (1,1595) | 1:782:A:ILE:HG23 | 1:788:A:GLY:H    | 11       | 0.21          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 17       | 0.21          |
| (1,1369) | 1:766:A:LEU:H    | 1:771:A:PHE:HD2  | 13       | 0.21          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD11 | 20       | 0.21          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD12 | 20       | 0.21          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD13 | 20       | 0.21          |
| (1,1149) | 1:743:A:ILE:HG21 | 1:747:A:GLN:HE22 | 17       | 0.21          |
| (1,1149) | 1:743:A:ILE:HG22 | 1:747:A:GLN:HE22 | 17       | 0.21          |
| (1,1149) | 1:743:A:ILE:HG23 | 1:747:A:GLN:HE22 | 17       | 0.21          |
| (1,1031) | 1:842:A:TYR:HD1  | 1:867:A:TYR:HD2  | 6        | 0.21          |
| (1,852)  | 1:842:A:TYR:HD1  | 1:867:A:TYR:HE2  | 11       | 0.21          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 1        | 0.21          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 1        | 0.21          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 1        | 0.21          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 1        | 0.21          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 1        | 0.21          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 1        | 0.21          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 1        | 0.21          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 1        | 0.21          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 1        | 0.21          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 7        | 0.21          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 7        | 0.21          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 7        | 0.21          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 11       | 0.21          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 11       | 0.21          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 11       | 0.21          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 17       | 0.21          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 17       | 0.21          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 17       | 0.21          |
| (1,561)  | 1:830:A:MET:HE1  | 1:879:A:TYR:HA   | 17       | 0.21          |
| (1,561)  | 1:830:A:MET:HE2  | 1:879:A:TYR:HA   | 17       | 0.21          |
| (1,561)  | 1:830:A:MET:HE3  | 1:879:A:TYR:HA   | 17       | 0.21          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 17       | 0.21          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 17       | 0.21          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 17       | 0.21          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 5        | 0.2           |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 5        | 0.2           |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 5        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 5        | 0.2           |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 5        | 0.2           |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 5        | 0.2           |
| (1,2038) | 1:836:A:LEU:HD11 | 1:848:A:LEU:H    | 1        | 0.2           |
| (1,2038) | 1:836:A:LEU:HD12 | 1:848:A:LEU:H    | 1        | 0.2           |
| (1,2038) | 1:836:A:LEU:HD13 | 1:848:A:LEU:H    | 1        | 0.2           |
| (1,1167) | 1:743:A:ILE:HG13 | 1:748:A:MET:H    | 3        | 0.2           |
| (1,825)  | 1:882:A:PHE:HD1  | 1:883:A:SER:HA   | 4        | 0.2           |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 7        | 0.2           |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 7        | 0.2           |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 7        | 0.2           |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 7        | 0.2           |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 7        | 0.2           |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 7        | 0.2           |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 7        | 0.2           |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 7        | 0.2           |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 7        | 0.2           |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 3        | 0.2           |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 3        | 0.2           |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 3        | 0.2           |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB1  | 20       | 0.2           |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB2  | 20       | 0.2           |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB3  | 20       | 0.2           |
| (1,116)  | 1:765:A:THR:HG21 | 1:771:A:PHE:HZ   | 13       | 0.2           |
| (1,116)  | 1:765:A:THR:HG22 | 1:771:A:PHE:HZ   | 13       | 0.2           |
| (1,116)  | 1:765:A:THR:HG23 | 1:771:A:PHE:HZ   | 13       | 0.2           |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 6        | 0.2           |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 6        | 0.2           |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 6        | 0.2           |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 11       | 0.2           |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 11       | 0.2           |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 11       | 0.2           |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 20       | 0.2           |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 20       | 0.2           |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 20       | 0.2           |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 11       | 0.19          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 11       | 0.19          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 11       | 0.19          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 11       | 0.19          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 11       | 0.19          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 11       | 0.19          |
| (1,2587) | 1:794:A:ARG:HD2  | 1:795:A:ILE:H    | 10       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2587) | 1:794:A:ARG:HD3  | 1:795:A:ILE:H    | 10       | 0.19          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 5        | 0.19          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 5        | 0.19          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 5        | 0.19          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 11       | 0.19          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 11       | 0.19          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 11       | 0.19          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 6        | 0.19          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 6        | 0.19          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 6        | 0.19          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 15       | 0.19          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 15       | 0.19          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 15       | 0.19          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 1        | 0.19          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 1        | 0.19          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 1        | 0.19          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 6        | 0.19          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 6        | 0.19          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 6        | 0.19          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 14       | 0.19          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 14       | 0.19          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 14       | 0.19          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 18       | 0.19          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 18       | 0.19          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 18       | 0.19          |
| (1,1595) | 1:782:A:ILE:HG21 | 1:788:A:GLY:H    | 20       | 0.19          |
| (1,1595) | 1:782:A:ILE:HG22 | 1:788:A:GLY:H    | 20       | 0.19          |
| (1,1595) | 1:782:A:ILE:HG23 | 1:788:A:GLY:H    | 20       | 0.19          |
| (1,1543) | 1:776:A:ILE:HD11 | 1:782:A:ILE:H    | 11       | 0.19          |
| (1,1543) | 1:776:A:ILE:HD12 | 1:782:A:ILE:H    | 11       | 0.19          |
| (1,1543) | 1:776:A:ILE:HD13 | 1:782:A:ILE:H    | 11       | 0.19          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 18       | 0.19          |
| (1,1486) | 1:775:A:LEU:HD11 | 1:776:A:ILE:H    | 9        | 0.19          |
| (1,1486) | 1:775:A:LEU:HD12 | 1:776:A:ILE:H    | 9        | 0.19          |
| (1,1486) | 1:775:A:LEU:HD13 | 1:776:A:ILE:H    | 9        | 0.19          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 1        | 0.19          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 1        | 0.19          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 1        | 0.19          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 1        | 0.19          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 1        | 0.19          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 1        | 0.19          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD11 | 1        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD12 | 1        | 0.19          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD13 | 1        | 0.19          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 18       | 0.19          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 1        | 0.19          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 1        | 0.19          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 1        | 0.19          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 14       | 0.19          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 14       | 0.19          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 14       | 0.19          |
| (1,571)  | 1:832:A:SER:HB2  | 1:835:A:ILE:HD11 | 17       | 0.19          |
| (1,571)  | 1:832:A:SER:HB2  | 1:835:A:ILE:HD12 | 17       | 0.19          |
| (1,571)  | 1:832:A:SER:HB2  | 1:835:A:ILE:HD13 | 17       | 0.19          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB1  | 7        | 0.19          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB2  | 7        | 0.19          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB3  | 7        | 0.19          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 9        | 0.19          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 9        | 0.19          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 9        | 0.19          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 14       | 0.19          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 14       | 0.19          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 14       | 0.19          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 6        | 0.18          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 6        | 0.18          |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 20       | 0.18          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 20       | 0.18          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 20       | 0.18          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 20       | 0.18          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 20       | 0.18          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 20       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 13       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 13       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 13       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 13       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 13       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 13       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 14       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 14       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 14       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 14       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 14       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 14       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 17       | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 17       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 17       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 17       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 17       | 0.18          |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 17       | 0.18          |
| (1,2522) | 1:885:A:ALA:HB1  | 1:886:A:LEU:H    | 17       | 0.18          |
| (1,2522) | 1:885:A:ALA:HB2  | 1:886:A:LEU:H    | 17       | 0.18          |
| (1,2522) | 1:885:A:ALA:HB3  | 1:886:A:LEU:H    | 17       | 0.18          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 9        | 0.18          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 9        | 0.18          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 9        | 0.18          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 14       | 0.18          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 14       | 0.18          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 14       | 0.18          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 5        | 0.18          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 5        | 0.18          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 5        | 0.18          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 9        | 0.18          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 9        | 0.18          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 9        | 0.18          |
| (1,1856) | 1:808:A:THR:HG21 | 1:810:A:GLN:H    | 11       | 0.18          |
| (1,1856) | 1:808:A:THR:HG22 | 1:810:A:GLN:H    | 11       | 0.18          |
| (1,1856) | 1:808:A:THR:HG23 | 1:810:A:GLN:H    | 11       | 0.18          |
| (1,1855) | 1:810:A:GLN:H    | 1:811:A:ALA:HB1  | 13       | 0.18          |
| (1,1855) | 1:810:A:GLN:H    | 1:811:A:ALA:HB2  | 13       | 0.18          |
| (1,1855) | 1:810:A:GLN:H    | 1:811:A:ALA:HB3  | 13       | 0.18          |
| (1,1644) | 1:792:A:PHE:H    | 1:794:A:ARG:HG2  | 10       | 0.18          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 3        | 0.18          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 16       | 0.18          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD11 | 11       | 0.18          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD12 | 11       | 0.18          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD13 | 11       | 0.18          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 4        | 0.18          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 4        | 0.18          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 4        | 0.18          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 4        | 0.18          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 4        | 0.18          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 4        | 0.18          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 4        | 0.18          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 4        | 0.18          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 4        | 0.18          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 5        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 5        | 0.18          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 5        | 0.18          |
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD21 | 13       | 0.18          |
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD22 | 13       | 0.18          |
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD23 | 13       | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 3        | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 3        | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 3        | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 4        | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 4        | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 4        | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 7        | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 7        | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 7        | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 10       | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 10       | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 10       | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 18       | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 18       | 0.18          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 18       | 0.18          |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD2  | 3        | 0.17          |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD3  | 3        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 6        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 6        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 6        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 6        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 6        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 6        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 8        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 8        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 8        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 8        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 8        | 0.17          |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 8        | 0.17          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 5        | 0.17          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 5        | 0.17          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 5        | 0.17          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 5        | 0.17          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 5        | 0.17          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 5        | 0.17          |
| (1,2591) | 1:803:A:ARG:H    | 1:803:A:ARG:HG2  | 1        | 0.17          |
| (1,2591) | 1:803:A:ARG:H    | 1:803:A:ARG:HG3  | 1        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 5        | 0.17          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 5        | 0.17          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 5        | 0.17          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 11       | 0.17          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 11       | 0.17          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 11       | 0.17          |
| (1,1971) | 1:820:A:THR:HG21 | 1:821:A:ALA:H    | 5        | 0.17          |
| (1,1971) | 1:820:A:THR:HG22 | 1:821:A:ALA:H    | 5        | 0.17          |
| (1,1971) | 1:820:A:THR:HG23 | 1:821:A:ALA:H    | 5        | 0.17          |
| (1,1971) | 1:820:A:THR:HG21 | 1:821:A:ALA:H    | 18       | 0.17          |
| (1,1971) | 1:820:A:THR:HG22 | 1:821:A:ALA:H    | 18       | 0.17          |
| (1,1971) | 1:820:A:THR:HG23 | 1:821:A:ALA:H    | 18       | 0.17          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 7        | 0.17          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 7        | 0.17          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 7        | 0.17          |
| (1,1595) | 1:782:A:ILE:HG21 | 1:788:A:GLY:H    | 1        | 0.17          |
| (1,1595) | 1:782:A:ILE:HG22 | 1:788:A:GLY:H    | 1        | 0.17          |
| (1,1595) | 1:782:A:ILE:HG23 | 1:788:A:GLY:H    | 1        | 0.17          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 4        | 0.17          |
| (1,1122) | 1:745:A:GLN:HB2  | 1:745:A:GLN:HE22 | 4        | 0.17          |
| (1,1118) | 1:743:A:ILE:HG13 | 1:744:A:SER:H    | 3        | 0.17          |
| (1,1118) | 1:743:A:ILE:HG13 | 1:744:A:SER:H    | 11       | 0.17          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 15       | 0.17          |
| (1,825)  | 1:882:A:PHE:HD1  | 1:883:A:SER:HA   | 18       | 0.17          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 18       | 0.17          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 18       | 0.17          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 18       | 0.17          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 18       | 0.17          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 18       | 0.17          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 18       | 0.17          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 18       | 0.17          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 18       | 0.17          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 18       | 0.17          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 15       | 0.17          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 15       | 0.17          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 15       | 0.17          |
| (1,307)  | 1:785:A:ASP:HB3  | 1:787:A:GLN:H    | 10       | 0.17          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 4        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 4        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 4        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 4        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 4        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 4        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 7        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 7        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 7        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 7        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 7        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 7        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 9        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 9        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 9        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 9        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 9        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 9        | 0.16          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 16       | 0.16          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 16       | 0.16          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 16       | 0.16          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 16       | 0.16          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 16       | 0.16          |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 16       | 0.16          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 14       | 0.16          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 14       | 0.16          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 14       | 0.16          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 14       | 0.16          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 14       | 0.16          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 14       | 0.16          |
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG11 | 12       | 0.16          |
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG12 | 12       | 0.16          |
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG13 | 12       | 0.16          |
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG21 | 12       | 0.16          |
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG22 | 12       | 0.16          |
| (1,2623) | 1:826:A:ALA:HA   | 1:829:A:VAL:HG23 | 12       | 0.16          |
| (1,2587) | 1:794:A:ARG:HD2  | 1:795:A:ILE:H    | 1        | 0.16          |
| (1,2587) | 1:794:A:ARG:HD3  | 1:795:A:ILE:H    | 1        | 0.16          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 20       | 0.16          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 20       | 0.16          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 20       | 0.16          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 4        | 0.16          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 4        | 0.16          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 4        | 0.16          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 10       | 0.16          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 10       | 0.16          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 10       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 20       | 0.16          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 20       | 0.16          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 20       | 0.16          |
| (1,2072) | 1:838:A:GLY:H    | 1:839:A:ASP:HA   | 9        | 0.16          |
| (1,1971) | 1:820:A:THR:HG21 | 1:821:A:ALA:H    | 19       | 0.16          |
| (1,1971) | 1:820:A:THR:HG22 | 1:821:A:ALA:H    | 19       | 0.16          |
| (1,1971) | 1:820:A:THR:HG23 | 1:821:A:ALA:H    | 19       | 0.16          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 1        | 0.16          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 1        | 0.16          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 1        | 0.16          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 4        | 0.16          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 4        | 0.16          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 4        | 0.16          |
| (1,1856) | 1:808:A:THR:HG21 | 1:810:A:GLN:H    | 5        | 0.16          |
| (1,1856) | 1:808:A:THR:HG22 | 1:810:A:GLN:H    | 5        | 0.16          |
| (1,1856) | 1:808:A:THR:HG23 | 1:810:A:GLN:H    | 5        | 0.16          |
| (1,1856) | 1:808:A:THR:HG21 | 1:810:A:GLN:H    | 17       | 0.16          |
| (1,1856) | 1:808:A:THR:HG22 | 1:810:A:GLN:H    | 17       | 0.16          |
| (1,1856) | 1:808:A:THR:HG23 | 1:810:A:GLN:H    | 17       | 0.16          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 2        | 0.16          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 2        | 0.16          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 2        | 0.16          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 19       | 0.16          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 19       | 0.16          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 19       | 0.16          |
| (1,1671) | 1:794:A:ARG:HG2  | 1:795:A:ILE:H    | 6        | 0.16          |
| (1,1595) | 1:782:A:ILE:HG21 | 1:788:A:GLY:H    | 18       | 0.16          |
| (1,1595) | 1:782:A:ILE:HG22 | 1:788:A:GLY:H    | 18       | 0.16          |
| (1,1595) | 1:782:A:ILE:HG23 | 1:788:A:GLY:H    | 18       | 0.16          |
| (1,1486) | 1:775:A:LEU:HD11 | 1:776:A:ILE:H    | 5        | 0.16          |
| (1,1486) | 1:775:A:LEU:HD12 | 1:776:A:ILE:H    | 5        | 0.16          |
| (1,1486) | 1:775:A:LEU:HD13 | 1:776:A:ILE:H    | 5        | 0.16          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 11       | 0.16          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 11       | 0.16          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 11       | 0.16          |
| (1,1120) | 1:743:A:ILE:HD11 | 1:744:A:SER:H    | 11       | 0.16          |
| (1,1120) | 1:743:A:ILE:HD12 | 1:744:A:SER:H    | 11       | 0.16          |
| (1,1120) | 1:743:A:ILE:HD13 | 1:744:A:SER:H    | 11       | 0.16          |
| (1,962)  | 1:812:A:PHE:HD1  | 1:816:A:MET:HA   | 13       | 0.16          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 13       | 0.16          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 13       | 0.16          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 13       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,561)  | 1:830:A:MET:HE1  | 1:879:A:TYR:HA   | 11       | 0.16          |
| (1,561)  | 1:830:A:MET:HE2  | 1:879:A:TYR:HA   | 11       | 0.16          |
| (1,561)  | 1:830:A:MET:HE3  | 1:879:A:TYR:HA   | 11       | 0.16          |
| (1,116)  | 1:765:A:THR:HG21 | 1:771:A:PHE:HZ   | 1        | 0.16          |
| (1,116)  | 1:765:A:THR:HG22 | 1:771:A:PHE:HZ   | 1        | 0.16          |
| (1,116)  | 1:765:A:THR:HG23 | 1:771:A:PHE:HZ   | 1        | 0.16          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 5        | 0.16          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 5        | 0.16          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 5        | 0.16          |
| (1,2716) | 1:887:A:TYR:HE2  | 1:888:A:GLY:HA2  | 18       | 0.15          |
| (1,2716) | 1:887:A:TYR:HE2  | 1:888:A:GLY:HA3  | 18       | 0.15          |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD2  | 9        | 0.15          |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD3  | 9        | 0.15          |
| (1,2644) | 1:834:A:LYS:HE2  | 1:879:A:TYR:HE2  | 17       | 0.15          |
| (1,2644) | 1:834:A:LYS:HE3  | 1:879:A:TYR:HE2  | 17       | 0.15          |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 3        | 0.15          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 3        | 0.15          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 3        | 0.15          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 3        | 0.15          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 3        | 0.15          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 3        | 0.15          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 3        | 0.15          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 3        | 0.15          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 3        | 0.15          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 3        | 0.15          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 3        | 0.15          |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 3        | 0.15          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG11 | 18       | 0.15          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG12 | 18       | 0.15          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG13 | 18       | 0.15          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG21 | 18       | 0.15          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG22 | 18       | 0.15          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG23 | 18       | 0.15          |
| (1,2507) | 1:887:A:TYR:H    | 1:889:A:GLU:H    | 13       | 0.15          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 14       | 0.15          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 14       | 0.15          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 14       | 0.15          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 18       | 0.15          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 18       | 0.15          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 18       | 0.15          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 17       | 0.15          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 17       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 17       | 0.15          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB1  | 3        | 0.15          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB2  | 3        | 0.15          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB3  | 3        | 0.15          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB1  | 18       | 0.15          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB2  | 18       | 0.15          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB3  | 18       | 0.15          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 6        | 0.15          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 6        | 0.15          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 6        | 0.15          |
| (1,1798) | 1:800:A:ASP:HB3  | 1:806:A:VAL:H    | 13       | 0.15          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 12       | 0.15          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 13       | 0.15          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 13       | 0.15          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 13       | 0.15          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 13       | 0.15          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 13       | 0.15          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 13       | 0.15          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD11 | 10       | 0.15          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD12 | 10       | 0.15          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD13 | 10       | 0.15          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD11 | 14       | 0.15          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD12 | 14       | 0.15          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD13 | 14       | 0.15          |
| (1,1167) | 1:743:A:ILE:HG13 | 1:748:A:MET:H    | 10       | 0.15          |
| (1,1149) | 1:743:A:ILE:HG21 | 1:747:A:GLN:HE22 | 9        | 0.15          |
| (1,1149) | 1:743:A:ILE:HG22 | 1:747:A:GLN:HE22 | 9        | 0.15          |
| (1,1149) | 1:743:A:ILE:HG23 | 1:747:A:GLN:HE22 | 9        | 0.15          |
| (1,1120) | 1:743:A:ILE:HD11 | 1:744:A:SER:H    | 3        | 0.15          |
| (1,1120) | 1:743:A:ILE:HD12 | 1:744:A:SER:H    | 3        | 0.15          |
| (1,1120) | 1:743:A:ILE:HD13 | 1:744:A:SER:H    | 3        | 0.15          |
| (1,1118) | 1:743:A:ILE:HG13 | 1:744:A:SER:H    | 10       | 0.15          |
| (1,1112) | 1:744:A:SER:H    | 1:747:A:GLN:HE21 | 13       | 0.15          |
| (1,1068) | 1:838:A:GLY:HA2  | 1:879:A:TYR:HE1  | 9        | 0.15          |
| (1,1068) | 1:838:A:GLY:HA2  | 1:879:A:TYR:HE1  | 17       | 0.15          |
| (1,965)  | 1:792:A:PHE:HD1  | 1:795:A:ILE:HD11 | 17       | 0.15          |
| (1,965)  | 1:792:A:PHE:HD1  | 1:795:A:ILE:HD12 | 17       | 0.15          |
| (1,965)  | 1:792:A:PHE:HD1  | 1:795:A:ILE:HD13 | 17       | 0.15          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 10       | 0.15          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 10       | 0.15          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 10       | 0.15          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 10       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 10       | 0.15          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 10       | 0.15          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 10       | 0.15          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 10       | 0.15          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 10       | 0.15          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 15       | 0.15          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 15       | 0.15          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 15       | 0.15          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 15       | 0.15          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 15       | 0.15          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 15       | 0.15          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 15       | 0.15          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 15       | 0.15          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 15       | 0.15          |
| (1,764)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HB2  | 1        | 0.15          |
| (1,764)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HB2  | 1        | 0.15          |
| (1,764)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HB2  | 1        | 0.15          |
| (1,764)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HB2  | 14       | 0.15          |
| (1,764)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HB2  | 14       | 0.15          |
| (1,764)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HB2  | 14       | 0.15          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB1  | 4        | 0.15          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB2  | 4        | 0.15          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB3  | 4        | 0.15          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 8        | 0.15          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 8        | 0.15          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 8        | 0.15          |
| (1,2720) | 1:890:A:SER:HB2  | 1:892:A:LEU:H    | 1        | 0.14          |
| (1,2720) | 1:890:A:SER:HB3  | 1:892:A:LEU:H    | 1        | 0.14          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 5        | 0.14          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 5        | 0.14          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 15       | 0.14          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 15       | 0.14          |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD2  | 5        | 0.14          |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD3  | 5        | 0.14          |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD2  | 13       | 0.14          |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD3  | 13       | 0.14          |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 6        | 0.14          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 6        | 0.14          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 6        | 0.14          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 6        | 0.14          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 6        | 0.14          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 6        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 7        | 0.14          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 7        | 0.14          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 7        | 0.14          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 7        | 0.14          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 7        | 0.14          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 7        | 0.14          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 19       | 0.14          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 19       | 0.14          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 19       | 0.14          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 19       | 0.14          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 19       | 0.14          |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 19       | 0.14          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 8        | 0.14          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 8        | 0.14          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 8        | 0.14          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 8        | 0.14          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 8        | 0.14          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 8        | 0.14          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG11 | 13       | 0.14          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG12 | 13       | 0.14          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG13 | 13       | 0.14          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG21 | 13       | 0.14          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG22 | 13       | 0.14          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG23 | 13       | 0.14          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG11 | 12       | 0.14          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG12 | 12       | 0.14          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG13 | 12       | 0.14          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG21 | 12       | 0.14          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG22 | 12       | 0.14          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG23 | 12       | 0.14          |
| (1,2621) | 1:824:A:ASP:HB2  | 1:826:A:ALA:H    | 1        | 0.14          |
| (1,2621) | 1:824:A:ASP:HB3  | 1:826:A:ALA:H    | 1        | 0.14          |
| (1,2613) | 1:819:A:GLU:HB2  | 1:820:A:THR:H    | 8        | 0.14          |
| (1,2613) | 1:819:A:GLU:HB3  | 1:820:A:THR:H    | 8        | 0.14          |
| (1,2585) | 1:793:A:ALA:HB1  | 1:794:A:ARG:HD2  | 14       | 0.14          |
| (1,2585) | 1:793:A:ALA:HB1  | 1:794:A:ARG:HD3  | 14       | 0.14          |
| (1,2585) | 1:793:A:ALA:HB2  | 1:794:A:ARG:HD2  | 14       | 0.14          |
| (1,2585) | 1:793:A:ALA:HB2  | 1:794:A:ARG:HD3  | 14       | 0.14          |
| (1,2585) | 1:793:A:ALA:HB3  | 1:794:A:ARG:HD2  | 14       | 0.14          |
| (1,2585) | 1:793:A:ALA:HB3  | 1:794:A:ARG:HD3  | 14       | 0.14          |
| (1,2520) | 1:825:A:THR:H    | 1:826:A:ALA:HB1  | 15       | 0.14          |
| (1,2520) | 1:825:A:THR:H    | 1:826:A:ALA:HB2  | 15       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2520) | 1:825:A:THR:H    | 1:826:A:ALA:HB3  | 15       | 0.14          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 3        | 0.14          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 3        | 0.14          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 3        | 0.14          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 9        | 0.14          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 9        | 0.14          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 9        | 0.14          |
| (1,2383) | 1:869:A:GLY:H    | 1:873:A:VAL:H    | 13       | 0.14          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 19       | 0.14          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 19       | 0.14          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 19       | 0.14          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB1  | 9        | 0.14          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB2  | 9        | 0.14          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB3  | 9        | 0.14          |
| (1,2038) | 1:836:A:LEU:HD11 | 1:848:A:LEU:H    | 13       | 0.14          |
| (1,2038) | 1:836:A:LEU:HD12 | 1:848:A:LEU:H    | 13       | 0.14          |
| (1,2038) | 1:836:A:LEU:HD13 | 1:848:A:LEU:H    | 13       | 0.14          |
| (1,2014) | 1:785:A:ASP:H    | 1:789:A:GLU:HG2  | 11       | 0.14          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 20       | 0.14          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 20       | 0.14          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 20       | 0.14          |
| (1,1856) | 1:808:A:THR:HG21 | 1:810:A:GLN:H    | 3        | 0.14          |
| (1,1856) | 1:808:A:THR:HG22 | 1:810:A:GLN:H    | 3        | 0.14          |
| (1,1856) | 1:808:A:THR:HG23 | 1:810:A:GLN:H    | 3        | 0.14          |
| (1,1849) | 1:810:A:GLN:H    | 1:812:A:PHE:HE2  | 13       | 0.14          |
| (1,1543) | 1:776:A:ILE:HD11 | 1:782:A:ILE:H    | 10       | 0.14          |
| (1,1543) | 1:776:A:ILE:HD12 | 1:782:A:ILE:H    | 10       | 0.14          |
| (1,1543) | 1:776:A:ILE:HD13 | 1:782:A:ILE:H    | 10       | 0.14          |
| (1,1492) | 1:798:A:ILE:HA   | 1:800:A:ASP:H    | 13       | 0.14          |
| (1,1486) | 1:775:A:LEU:HD11 | 1:776:A:ILE:H    | 6        | 0.14          |
| (1,1486) | 1:775:A:LEU:HD12 | 1:776:A:ILE:H    | 6        | 0.14          |
| (1,1486) | 1:775:A:LEU:HD13 | 1:776:A:ILE:H    | 6        | 0.14          |
| (1,1486) | 1:775:A:LEU:HD11 | 1:776:A:ILE:H    | 7        | 0.14          |
| (1,1486) | 1:775:A:LEU:HD12 | 1:776:A:ILE:H    | 7        | 0.14          |
| (1,1486) | 1:775:A:LEU:HD13 | 1:776:A:ILE:H    | 7        | 0.14          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 11       | 0.14          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 11       | 0.14          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 11       | 0.14          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD11 | 5        | 0.14          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD12 | 5        | 0.14          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD13 | 5        | 0.14          |
| (1,1167) | 1:743:A:ILE:HG13 | 1:748:A:MET:H    | 13       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1149) | 1:743:A:ILE:HG21 | 1:747:A:GLN:HE22 | 13       | 0.14          |
| (1,1149) | 1:743:A:ILE:HG22 | 1:747:A:GLN:HE22 | 13       | 0.14          |
| (1,1149) | 1:743:A:ILE:HG23 | 1:747:A:GLN:HE22 | 13       | 0.14          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 12       | 0.14          |
| (1,950)  | 1:775:A:LEU:HB2  | 1:780:A:TYR:HD1  | 16       | 0.14          |
| (1,689)  | 1:852:A:LEU:H    | 1:852:A:LEU:HD21 | 1        | 0.14          |
| (1,689)  | 1:852:A:LEU:H    | 1:852:A:LEU:HD22 | 1        | 0.14          |
| (1,689)  | 1:852:A:LEU:H    | 1:852:A:LEU:HD23 | 1        | 0.14          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 6        | 0.14          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 6        | 0.14          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 6        | 0.14          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 16       | 0.14          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 16       | 0.14          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 16       | 0.14          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 18       | 0.14          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 18       | 0.14          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 18       | 0.14          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB1  | 9        | 0.14          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB2  | 9        | 0.14          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB3  | 9        | 0.14          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB1  | 10       | 0.14          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB2  | 10       | 0.14          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB3  | 10       | 0.14          |
| (1,251)  | 1:773:A:ALA:HA   | 1:776:A:ILE:HG21 | 9        | 0.14          |
| (1,251)  | 1:773:A:ALA:HA   | 1:776:A:ILE:HG22 | 9        | 0.14          |
| (1,251)  | 1:773:A:ALA:HA   | 1:776:A:ILE:HG23 | 9        | 0.14          |
| (1,116)  | 1:765:A:THR:HG21 | 1:771:A:PHE:HZ   | 3        | 0.14          |
| (1,116)  | 1:765:A:THR:HG22 | 1:771:A:PHE:HZ   | 3        | 0.14          |
| (1,116)  | 1:765:A:THR:HG23 | 1:771:A:PHE:HZ   | 3        | 0.14          |
| (1,116)  | 1:765:A:THR:HG21 | 1:771:A:PHE:HZ   | 17       | 0.14          |
| (1,116)  | 1:765:A:THR:HG22 | 1:771:A:PHE:HZ   | 17       | 0.14          |
| (1,116)  | 1:765:A:THR:HG23 | 1:771:A:PHE:HZ   | 17       | 0.14          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 15       | 0.14          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 15       | 0.14          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 15       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD11 | 1:748:A:MET:HE1  | 13       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD11 | 1:748:A:MET:HE2  | 13       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD11 | 1:748:A:MET:HE3  | 13       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD12 | 1:748:A:MET:HE1  | 13       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD12 | 1:748:A:MET:HE2  | 13       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD12 | 1:748:A:MET:HE3  | 13       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD13 | 1:748:A:MET:HE1  | 13       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,43)   | 1:743:A:ILE:HD13 | 1:748:A:MET:HE2  | 13       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD13 | 1:748:A:MET:HE3  | 13       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD11 | 1:748:A:MET:HE1  | 17       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD11 | 1:748:A:MET:HE2  | 17       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD11 | 1:748:A:MET:HE3  | 17       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD12 | 1:748:A:MET:HE1  | 17       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD12 | 1:748:A:MET:HE2  | 17       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD12 | 1:748:A:MET:HE3  | 17       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD13 | 1:748:A:MET:HE1  | 17       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD13 | 1:748:A:MET:HE2  | 17       | 0.14          |
| (1,43)   | 1:743:A:ILE:HD13 | 1:748:A:MET:HE3  | 17       | 0.14          |
| (1,25)   | 1:746:A:GLU:HG3  | 1:747:A:GLN:H    | 13       | 0.14          |
| (1,12)   | 1:798:A:ILE:HG21 | 1:800:A:ASP:H    | 13       | 0.14          |
| (1,12)   | 1:798:A:ILE:HG22 | 1:800:A:ASP:H    | 13       | 0.14          |
| (1,12)   | 1:798:A:ILE:HG23 | 1:800:A:ASP:H    | 13       | 0.14          |
| (1,9)    | 1:743:A:ILE:HD11 | 1:747:A:GLN:HA   | 1        | 0.14          |
| (1,9)    | 1:743:A:ILE:HD12 | 1:747:A:GLN:HA   | 1        | 0.14          |
| (1,9)    | 1:743:A:ILE:HD13 | 1:747:A:GLN:HA   | 1        | 0.14          |
| (1,8)    | 1:743:A:ILE:HD11 | 1:748:A:MET:HG2  | 13       | 0.14          |
| (1,8)    | 1:743:A:ILE:HD12 | 1:748:A:MET:HG2  | 13       | 0.14          |
| (1,8)    | 1:743:A:ILE:HD13 | 1:748:A:MET:HG2  | 13       | 0.14          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 9        | 0.13          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 9        | 0.13          |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD2  | 18       | 0.13          |
| (1,2677) | 1:850:A:ARG:HA   | 1:850:A:ARG:HD3  | 18       | 0.13          |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 8        | 0.13          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 8        | 0.13          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 8        | 0.13          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 8        | 0.13          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 8        | 0.13          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 8        | 0.13          |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 12       | 0.13          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 12       | 0.13          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 12       | 0.13          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 12       | 0.13          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 12       | 0.13          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 12       | 0.13          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 16       | 0.13          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 16       | 0.13          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 16       | 0.13          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 16       | 0.13          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 16       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 16       | 0.13          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 19       | 0.13          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 19       | 0.13          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 19       | 0.13          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 19       | 0.13          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 19       | 0.13          |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 19       | 0.13          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG11 | 5        | 0.13          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG12 | 5        | 0.13          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG13 | 5        | 0.13          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG21 | 5        | 0.13          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG22 | 5        | 0.13          |
| (1,2626) | 1:828:A:GLN:HG3  | 1:829:A:VAL:HG23 | 5        | 0.13          |
| (1,2465) | 1:830:A:MET:HE1  | 1:881:A:SER:H    | 13       | 0.13          |
| (1,2465) | 1:830:A:MET:HE2  | 1:881:A:SER:H    | 13       | 0.13          |
| (1,2465) | 1:830:A:MET:HE3  | 1:881:A:SER:H    | 13       | 0.13          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 12       | 0.13          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 12       | 0.13          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 12       | 0.13          |
| (1,2351) | 1:865:A:ALA:H    | 1:866:A:PRO:HD3  | 13       | 0.13          |
| (1,2325) | 1:861:A:ILE:HD11 | 1:862:A:ALA:H    | 10       | 0.13          |
| (1,2325) | 1:861:A:ILE:HD12 | 1:862:A:ALA:H    | 10       | 0.13          |
| (1,2325) | 1:861:A:ILE:HD13 | 1:862:A:ALA:H    | 10       | 0.13          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 11       | 0.13          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 11       | 0.13          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 11       | 0.13          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 3        | 0.13          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 3        | 0.13          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 3        | 0.13          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 12       | 0.13          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 12       | 0.13          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 12       | 0.13          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 11       | 0.13          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 11       | 0.13          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 11       | 0.13          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 14       | 0.13          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 14       | 0.13          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 14       | 0.13          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 18       | 0.13          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 18       | 0.13          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 18       | 0.13          |
| (1,1892) | 1:765:A:THR:HG21 | 1:811:A:ALA:H    | 13       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1892) | 1:765:A:THR:HG22 | 1:811:A:ALA:H    | 13       | 0.13          |
| (1,1892) | 1:765:A:THR:HG23 | 1:811:A:ALA:H    | 13       | 0.13          |
| (1,1875) | 1:810:A:GLN:HG3  | 1:810:A:GLN:HE22 | 13       | 0.13          |
| (1,1671) | 1:794:A:ARG:HG2  | 1:795:A:ILE:H    | 15       | 0.13          |
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG21 | 13       | 0.13          |
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG22 | 13       | 0.13          |
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG23 | 13       | 0.13          |
| (1,1632) | 1:791:A:GLU:H    | 1:794:A:ARG:HG2  | 15       | 0.13          |
| (1,1595) | 1:782:A:ILE:HG21 | 1:788:A:GLY:H    | 13       | 0.13          |
| (1,1595) | 1:782:A:ILE:HG22 | 1:788:A:GLY:H    | 13       | 0.13          |
| (1,1595) | 1:782:A:ILE:HG23 | 1:788:A:GLY:H    | 13       | 0.13          |
| (1,1554) | 1:772:A:LYS:HD2  | 1:783:A:GLY:H    | 5        | 0.13          |
| (1,1543) | 1:776:A:ILE:HD11 | 1:782:A:ILE:H    | 17       | 0.13          |
| (1,1543) | 1:776:A:ILE:HD12 | 1:782:A:ILE:H    | 17       | 0.13          |
| (1,1543) | 1:776:A:ILE:HD13 | 1:782:A:ILE:H    | 17       | 0.13          |
| (1,1543) | 1:776:A:ILE:HD11 | 1:782:A:ILE:H    | 20       | 0.13          |
| (1,1543) | 1:776:A:ILE:HD12 | 1:782:A:ILE:H    | 20       | 0.13          |
| (1,1543) | 1:776:A:ILE:HD13 | 1:782:A:ILE:H    | 20       | 0.13          |
| (1,1527) | 1:775:A:LEU:HD11 | 1:780:A:TYR:H    | 13       | 0.13          |
| (1,1527) | 1:775:A:LEU:HD12 | 1:780:A:TYR:H    | 13       | 0.13          |
| (1,1527) | 1:775:A:LEU:HD13 | 1:780:A:TYR:H    | 13       | 0.13          |
| (1,1490) | 1:776:A:ILE:HG21 | 1:777:A:SER:H    | 1        | 0.13          |
| (1,1490) | 1:776:A:ILE:HG22 | 1:777:A:SER:H    | 1        | 0.13          |
| (1,1490) | 1:776:A:ILE:HG23 | 1:777:A:SER:H    | 1        | 0.13          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 9        | 0.13          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 9        | 0.13          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 9        | 0.13          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 4        | 0.13          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 4        | 0.13          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 4        | 0.13          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 14       | 0.13          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 14       | 0.13          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 14       | 0.13          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD11 | 6        | 0.13          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD12 | 6        | 0.13          |
| (1,1280) | 1:756:A:ASN:H    | 1:766:A:LEU:HD13 | 6        | 0.13          |
| (1,1118) | 1:743:A:ILE:HG13 | 1:744:A:SER:H    | 7        | 0.13          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 3        | 0.13          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 3        | 0.13          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 3        | 0.13          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 3        | 0.13          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 3        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 3        | 0.13          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 3        | 0.13          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 3        | 0.13          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 3        | 0.13          |
| (1,764)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HB2  | 5        | 0.13          |
| (1,764)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HB2  | 5        | 0.13          |
| (1,764)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HB2  | 5        | 0.13          |
| (1,764)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HB2  | 9        | 0.13          |
| (1,764)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HB2  | 9        | 0.13          |
| (1,764)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HB2  | 9        | 0.13          |
| (1,764)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HB2  | 10       | 0.13          |
| (1,764)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HB2  | 10       | 0.13          |
| (1,764)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HB2  | 10       | 0.13          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 4        | 0.13          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 4        | 0.13          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 4        | 0.13          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 10       | 0.13          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 10       | 0.13          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 10       | 0.13          |
| (1,572)  | 1:832:A:SER:HB3  | 1:835:A:ILE:HD11 | 9        | 0.13          |
| (1,572)  | 1:832:A:SER:HB3  | 1:835:A:ILE:HD12 | 9        | 0.13          |
| (1,572)  | 1:832:A:SER:HB3  | 1:835:A:ILE:HD13 | 9        | 0.13          |
| (1,571)  | 1:832:A:SER:HB2  | 1:835:A:ILE:HD11 | 5        | 0.13          |
| (1,571)  | 1:832:A:SER:HB2  | 1:835:A:ILE:HD12 | 5        | 0.13          |
| (1,571)  | 1:832:A:SER:HB2  | 1:835:A:ILE:HD13 | 5        | 0.13          |
| (1,561)  | 1:830:A:MET:HE1  | 1:879:A:TYR:HA   | 15       | 0.13          |
| (1,561)  | 1:830:A:MET:HE2  | 1:879:A:TYR:HA   | 15       | 0.13          |
| (1,561)  | 1:830:A:MET:HE3  | 1:879:A:TYR:HA   | 15       | 0.13          |
| (1,134)  | 1:766:A:LEU:HG   | 1:771:A:PHE:H    | 13       | 0.13          |
| (1,116)  | 1:765:A:THR:HG21 | 1:771:A:PHE:HZ   | 9        | 0.13          |
| (1,116)  | 1:765:A:THR:HG22 | 1:771:A:PHE:HZ   | 9        | 0.13          |
| (1,116)  | 1:765:A:THR:HG23 | 1:771:A:PHE:HZ   | 9        | 0.13          |
| (1,50)   | 1:743:A:ILE:HD11 | 1:748:A:MET:HG3  | 17       | 0.13          |
| (1,50)   | 1:743:A:ILE:HD12 | 1:748:A:MET:HG3  | 17       | 0.13          |
| (1,50)   | 1:743:A:ILE:HD13 | 1:748:A:MET:HG3  | 17       | 0.13          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB2  | 16       | 0.12          |
| (1,2694) | 1:867:A:TYR:HE1  | 1:871:A:ASP:HB3  | 16       | 0.12          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 11       | 0.12          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 11       | 0.12          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 11       | 0.12          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 11       | 0.12          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 11       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 11       | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG11 | 2        | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG12 | 2        | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG13 | 2        | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG21 | 2        | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG22 | 2        | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG23 | 2        | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG11 | 20       | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG12 | 20       | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG13 | 20       | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG21 | 20       | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG22 | 20       | 0.12          |
| (1,2622) | 1:826:A:ALA:H    | 1:829:A:VAL:HG23 | 20       | 0.12          |
| (1,2591) | 1:803:A:ARG:H    | 1:803:A:ARG:HG2  | 20       | 0.12          |
| (1,2591) | 1:803:A:ARG:H    | 1:803:A:ARG:HG3  | 20       | 0.12          |
| (1,2455) | 1:843:A:ILE:HD11 | 1:880:A:MET:H    | 7        | 0.12          |
| (1,2455) | 1:843:A:ILE:HD12 | 1:880:A:MET:H    | 7        | 0.12          |
| (1,2455) | 1:843:A:ILE:HD13 | 1:880:A:MET:H    | 7        | 0.12          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 5        | 0.12          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 5        | 0.12          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 5        | 0.12          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 4        | 0.12          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 4        | 0.12          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 4        | 0.12          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 13       | 0.12          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 13       | 0.12          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 13       | 0.12          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 8        | 0.12          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 8        | 0.12          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 8        | 0.12          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 15       | 0.12          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 15       | 0.12          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 15       | 0.12          |
| (1,2071) | 1:838:A:GLY:H    | 1:879:A:TYR:HE1  | 13       | 0.12          |
| (1,2063) | 1:835:A:ILE:H    | 1:837:A:ALA:H    | 17       | 0.12          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB1  | 11       | 0.12          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB2  | 11       | 0.12          |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB3  | 11       | 0.12          |
| (1,2038) | 1:836:A:LEU:HD11 | 1:848:A:LEU:H    | 11       | 0.12          |
| (1,2038) | 1:836:A:LEU:HD12 | 1:848:A:LEU:H    | 11       | 0.12          |
| (1,2038) | 1:836:A:LEU:HD13 | 1:848:A:LEU:H    | 11       | 0.12          |
| (1,2008) | 1:827:A:ASP:HB2  | 1:828:A:GLN:H    | 12       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 8        | 0.12          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 8        | 0.12          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 8        | 0.12          |
| (1,1937) | 1:799:A:VAL:HG11 | 1:815:A:PHE:H    | 13       | 0.12          |
| (1,1937) | 1:799:A:VAL:HG12 | 1:815:A:PHE:H    | 13       | 0.12          |
| (1,1937) | 1:799:A:VAL:HG13 | 1:815:A:PHE:H    | 13       | 0.12          |
| (1,1892) | 1:765:A:THR:HG21 | 1:811:A:ALA:H    | 4        | 0.12          |
| (1,1892) | 1:765:A:THR:HG22 | 1:811:A:ALA:H    | 4        | 0.12          |
| (1,1892) | 1:765:A:THR:HG23 | 1:811:A:ALA:H    | 4        | 0.12          |
| (1,1856) | 1:808:A:THR:HG21 | 1:810:A:GLN:H    | 9        | 0.12          |
| (1,1856) | 1:808:A:THR:HG22 | 1:810:A:GLN:H    | 9        | 0.12          |
| (1,1856) | 1:808:A:THR:HG23 | 1:810:A:GLN:H    | 9        | 0.12          |
| (1,1674) | 1:795:A:ILE:H    | 1:796:A:MET:HG2  | 1        | 0.12          |
| (1,1601) | 1:789:A:GLU:H    | 1:789:A:GLU:HG3  | 13       | 0.12          |
| (1,1595) | 1:782:A:ILE:HG21 | 1:788:A:GLY:H    | 9        | 0.12          |
| (1,1595) | 1:782:A:ILE:HG22 | 1:788:A:GLY:H    | 9        | 0.12          |
| (1,1595) | 1:782:A:ILE:HG23 | 1:788:A:GLY:H    | 9        | 0.12          |
| (1,1543) | 1:776:A:ILE:HD11 | 1:782:A:ILE:H    | 18       | 0.12          |
| (1,1543) | 1:776:A:ILE:HD12 | 1:782:A:ILE:H    | 18       | 0.12          |
| (1,1543) | 1:776:A:ILE:HD13 | 1:782:A:ILE:H    | 18       | 0.12          |
| (1,1527) | 1:775:A:LEU:HD11 | 1:780:A:TYR:H    | 9        | 0.12          |
| (1,1527) | 1:775:A:LEU:HD12 | 1:780:A:TYR:H    | 9        | 0.12          |
| (1,1527) | 1:775:A:LEU:HD13 | 1:780:A:TYR:H    | 9        | 0.12          |
| (1,1492) | 1:798:A:ILE:HA   | 1:800:A:ASP:H    | 17       | 0.12          |
| (1,1490) | 1:776:A:ILE:HG21 | 1:777:A:SER:H    | 4        | 0.12          |
| (1,1490) | 1:776:A:ILE:HG22 | 1:777:A:SER:H    | 4        | 0.12          |
| (1,1490) | 1:776:A:ILE:HG23 | 1:777:A:SER:H    | 4        | 0.12          |
| (1,1490) | 1:776:A:ILE:HG21 | 1:777:A:SER:H    | 17       | 0.12          |
| (1,1490) | 1:776:A:ILE:HG22 | 1:777:A:SER:H    | 17       | 0.12          |
| (1,1490) | 1:776:A:ILE:HG23 | 1:777:A:SER:H    | 17       | 0.12          |
| (1,1490) | 1:776:A:ILE:HG21 | 1:777:A:SER:H    | 18       | 0.12          |
| (1,1490) | 1:776:A:ILE:HG22 | 1:777:A:SER:H    | 18       | 0.12          |
| (1,1490) | 1:776:A:ILE:HG23 | 1:777:A:SER:H    | 18       | 0.12          |
| (1,1486) | 1:775:A:LEU:HD11 | 1:776:A:ILE:H    | 4        | 0.12          |
| (1,1486) | 1:775:A:LEU:HD12 | 1:776:A:ILE:H    | 4        | 0.12          |
| (1,1486) | 1:775:A:LEU:HD13 | 1:776:A:ILE:H    | 4        | 0.12          |
| (1,1486) | 1:775:A:LEU:HD11 | 1:776:A:ILE:H    | 11       | 0.12          |
| (1,1486) | 1:775:A:LEU:HD12 | 1:776:A:ILE:H    | 11       | 0.12          |
| (1,1486) | 1:775:A:LEU:HD13 | 1:776:A:ILE:H    | 11       | 0.12          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 10       | 0.12          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 10       | 0.12          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 10       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 18       | 0.12          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 18       | 0.12          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 18       | 0.12          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 20       | 0.12          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 20       | 0.12          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 20       | 0.12          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 9        | 0.12          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 9        | 0.12          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 9        | 0.12          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 10       | 0.12          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 10       | 0.12          |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 10       | 0.12          |
| (1,1165) | 1:743:A:ILE:HB   | 1:748:A:MET:H    | 7        | 0.12          |
| (1,1149) | 1:743:A:ILE:HG21 | 1:747:A:GLN:HE22 | 11       | 0.12          |
| (1,1149) | 1:743:A:ILE:HG22 | 1:747:A:GLN:HE22 | 11       | 0.12          |
| (1,1149) | 1:743:A:ILE:HG23 | 1:747:A:GLN:HE22 | 11       | 0.12          |
| (1,1120) | 1:743:A:ILE:HD11 | 1:744:A:SER:H    | 5        | 0.12          |
| (1,1120) | 1:743:A:ILE:HD12 | 1:744:A:SER:H    | 5        | 0.12          |
| (1,1120) | 1:743:A:ILE:HD13 | 1:744:A:SER:H    | 5        | 0.12          |
| (1,1120) | 1:743:A:ILE:HD11 | 1:744:A:SER:H    | 10       | 0.12          |
| (1,1120) | 1:743:A:ILE:HD12 | 1:744:A:SER:H    | 10       | 0.12          |
| (1,1120) | 1:743:A:ILE:HD13 | 1:744:A:SER:H    | 10       | 0.12          |
| (1,1079) | 1:867:A:TYR:HD1  | 1:877:A:LEU:H    | 13       | 0.12          |
| (1,877)  | 1:743:A:ILE:HG13 | 1:751:A:PHE:HE2  | 7        | 0.12          |
| (1,764)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HB2  | 4        | 0.12          |
| (1,764)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HB2  | 4        | 0.12          |
| (1,764)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HB2  | 4        | 0.12          |
| (1,764)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HB2  | 18       | 0.12          |
| (1,764)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HB2  | 18       | 0.12          |
| (1,764)  | 1:865:A:ALA:HB3  | 1:882:A:PHE:HB2  | 18       | 0.12          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 2        | 0.12          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 2        | 0.12          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 2        | 0.12          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 8        | 0.12          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 8        | 0.12          |
| (1,599)  | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 8        | 0.12          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB1  | 2        | 0.12          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB2  | 2        | 0.12          |
| (1,534)  | 1:819:A:GLU:HA   | 1:821:A:ALA:HB3  | 2        | 0.12          |
| (1,251)  | 1:773:A:ALA:HA   | 1:776:A:ILE:HG21 | 17       | 0.12          |
| (1,251)  | 1:773:A:ALA:HA   | 1:776:A:ILE:HG22 | 17       | 0.12          |
| (1,251)  | 1:773:A:ALA:HA   | 1:776:A:ILE:HG23 | 17       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD21 | 6        | 0.12          |
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD22 | 6        | 0.12          |
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD23 | 6        | 0.12          |
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD21 | 7        | 0.12          |
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD22 | 7        | 0.12          |
| (1,228)  | 1:771:A:PHE:HA   | 1:775:A:LEU:HD23 | 7        | 0.12          |
| (1,134)  | 1:766:A:LEU:HG   | 1:771:A:PHE:H    | 1        | 0.12          |
| (1,134)  | 1:766:A:LEU:HG   | 1:771:A:PHE:H    | 17       | 0.12          |
| (1,116)  | 1:765:A:THR:HG21 | 1:771:A:PHE:HZ   | 10       | 0.12          |
| (1,116)  | 1:765:A:THR:HG22 | 1:771:A:PHE:HZ   | 10       | 0.12          |
| (1,116)  | 1:765:A:THR:HG23 | 1:771:A:PHE:HZ   | 10       | 0.12          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 2        | 0.12          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 2        | 0.12          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 2        | 0.12          |
| (1,2720) | 1:890:A:SER:HB2  | 1:892:A:LEU:H    | 14       | 0.11          |
| (1,2720) | 1:890:A:SER:HB3  | 1:892:A:LEU:H    | 14       | 0.11          |
| (1,2664) | 1:846:A:ASP:H    | 1:849:A:ARG:HB2  | 18       | 0.11          |
| (1,2664) | 1:846:A:ASP:H    | 1:849:A:ARG:HB3  | 18       | 0.11          |
| (1,2639) | 1:829:A:VAL:HG11 | 1:856:A:GLN:HE22 | 17       | 0.11          |
| (1,2639) | 1:829:A:VAL:HG12 | 1:856:A:GLN:HE22 | 17       | 0.11          |
| (1,2639) | 1:829:A:VAL:HG13 | 1:856:A:GLN:HE22 | 17       | 0.11          |
| (1,2639) | 1:829:A:VAL:HG21 | 1:856:A:GLN:HE22 | 17       | 0.11          |
| (1,2639) | 1:829:A:VAL:HG22 | 1:856:A:GLN:HE22 | 17       | 0.11          |
| (1,2639) | 1:829:A:VAL:HG23 | 1:856:A:GLN:HE22 | 17       | 0.11          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 10       | 0.11          |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 10       | 0.11          |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 10       | 0.11          |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 10       | 0.11          |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 10       | 0.11          |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 10       | 0.11          |
| (1,2585) | 1:793:A:ALA:HB1  | 1:794:A:ARG:HD2  | 13       | 0.11          |
| (1,2585) | 1:793:A:ALA:HB1  | 1:794:A:ARG:HD3  | 13       | 0.11          |
| (1,2585) | 1:793:A:ALA:HB2  | 1:794:A:ARG:HD2  | 13       | 0.11          |
| (1,2585) | 1:793:A:ALA:HB2  | 1:794:A:ARG:HD3  | 13       | 0.11          |
| (1,2585) | 1:793:A:ALA:HB3  | 1:794:A:ARG:HD2  | 13       | 0.11          |
| (1,2585) | 1:793:A:ALA:HB3  | 1:794:A:ARG:HD3  | 13       | 0.11          |
| (1,2452) | 1:837:A:ALA:HB1  | 1:880:A:MET:H    | 11       | 0.11          |
| (1,2452) | 1:837:A:ALA:HB2  | 1:880:A:MET:H    | 11       | 0.11          |
| (1,2452) | 1:837:A:ALA:HB3  | 1:880:A:MET:H    | 11       | 0.11          |
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 3        | 0.11          |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 3        | 0.11          |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 3        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 5        | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 5        | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 5        | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 6        | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 6        | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 6        | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 9        | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 9        | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 9        | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 14       | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 14       | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 14       | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 18       | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 18       | 0.11          |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 18       | 0.11          |
| (1,2269) | 1:858:A:GLU:H    | 1:858:A:GLU:HG3  | 17       | 0.11          |
| (1,2156) | 1:844:A:THR:HG21 | 1:845:A:MET:H    | 16       | 0.11          |
| (1,2156) | 1:844:A:THR:HG22 | 1:845:A:MET:H    | 16       | 0.11          |
| (1,2156) | 1:844:A:THR:HG23 | 1:845:A:MET:H    | 16       | 0.11          |
| (1,2131) | 1:842:A:TYR:HE2  | 1:844:A:THR:H    | 17       | 0.11          |
| (1,2099) | 1:841:A:ASN:HB2  | 1:841:A:ASN:HD22 | 3        | 0.11          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 8        | 0.11          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 8        | 0.11          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 8        | 0.11          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 10       | 0.11          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 10       | 0.11          |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 10       | 0.11          |
| (1,2074) | 1:836:A:LEU:HB3  | 1:838:A:GLY:H    | 17       | 0.11          |
| (1,2008) | 1:827:A:ASP:HB2  | 1:828:A:GLN:H    | 20       | 0.11          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 3        | 0.11          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 3        | 0.11          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 3        | 0.11          |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 15       | 0.11          |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 15       | 0.11          |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 15       | 0.11          |
| (1,1893) | 1:799:A:VAL:HG11 | 1:811:A:ALA:H    | 9        | 0.11          |
| (1,1893) | 1:799:A:VAL:HG12 | 1:811:A:ALA:H    | 9        | 0.11          |
| (1,1893) | 1:799:A:VAL:HG13 | 1:811:A:ALA:H    | 9        | 0.11          |
| (1,1893) | 1:799:A:VAL:HG11 | 1:811:A:ALA:H    | 11       | 0.11          |
| (1,1893) | 1:799:A:VAL:HG12 | 1:811:A:ALA:H    | 11       | 0.11          |
| (1,1893) | 1:799:A:VAL:HG13 | 1:811:A:ALA:H    | 11       | 0.11          |
| (1,1892) | 1:765:A:THR:HG21 | 1:811:A:ALA:H    | 14       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1892) | 1:765:A:THR:HG22 | 1:811:A:ALA:H    | 14       | 0.11          |
| (1,1892) | 1:765:A:THR:HG23 | 1:811:A:ALA:H    | 14       | 0.11          |
| (1,1883) | 1:808:A:THR:HA   | 1:811:A:ALA:H    | 13       | 0.11          |
| (1,1882) | 1:809:A:PHE:HD1  | 1:811:A:ALA:H    | 13       | 0.11          |
| (1,1841) | 1:808:A:THR:HG21 | 1:809:A:PHE:H    | 13       | 0.11          |
| (1,1841) | 1:808:A:THR:HG22 | 1:809:A:PHE:H    | 13       | 0.11          |
| (1,1841) | 1:808:A:THR:HG23 | 1:809:A:PHE:H    | 13       | 0.11          |
| (1,1827) | 1:808:A:THR:H    | 1:812:A:PHE:HB3  | 13       | 0.11          |
| (1,1798) | 1:800:A:ASP:HB3  | 1:806:A:VAL:H    | 6        | 0.11          |
| (1,1798) | 1:800:A:ASP:HB3  | 1:806:A:VAL:H    | 7        | 0.11          |
| (1,1798) | 1:800:A:ASP:HB3  | 1:806:A:VAL:H    | 9        | 0.11          |
| (1,1798) | 1:800:A:ASP:HB3  | 1:806:A:VAL:H    | 17       | 0.11          |
| (1,1742) | 1:802:A:ASN:H    | 1:804:A:LEU:HD21 | 13       | 0.11          |
| (1,1742) | 1:802:A:ASN:H    | 1:804:A:LEU:HD22 | 13       | 0.11          |
| (1,1742) | 1:802:A:ASN:H    | 1:804:A:LEU:HD23 | 13       | 0.11          |
| (1,1674) | 1:795:A:ILE:H    | 1:796:A:MET:HG2  | 5        | 0.11          |
| (1,1674) | 1:795:A:ILE:H    | 1:796:A:MET:HG2  | 10       | 0.11          |
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG21 | 9        | 0.11          |
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG22 | 9        | 0.11          |
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG23 | 9        | 0.11          |
| (1,1637) | 1:792:A:PHE:H    | 1:794:A:ARG:H    | 11       | 0.11          |
| (1,1601) | 1:789:A:GLU:H    | 1:789:A:GLU:HG3  | 16       | 0.11          |
| (1,1595) | 1:782:A:ILE:HG21 | 1:788:A:GLY:H    | 6        | 0.11          |
| (1,1595) | 1:782:A:ILE:HG22 | 1:788:A:GLY:H    | 6        | 0.11          |
| (1,1595) | 1:782:A:ILE:HG23 | 1:788:A:GLY:H    | 6        | 0.11          |
| (1,1595) | 1:782:A:ILE:HG21 | 1:788:A:GLY:H    | 8        | 0.11          |
| (1,1595) | 1:782:A:ILE:HG22 | 1:788:A:GLY:H    | 8        | 0.11          |
| (1,1595) | 1:782:A:ILE:HG23 | 1:788:A:GLY:H    | 8        | 0.11          |
| (1,1556) | 1:784:A:ASN:HA   | 1:785:A:ASP:H    | 11       | 0.11          |
| (1,1543) | 1:776:A:ILE:HD11 | 1:782:A:ILE:H    | 5        | 0.11          |
| (1,1543) | 1:776:A:ILE:HD12 | 1:782:A:ILE:H    | 5        | 0.11          |
| (1,1543) | 1:776:A:ILE:HD13 | 1:782:A:ILE:H    | 5        | 0.11          |
| (1,1512) | 1:775:A:LEU:HB2  | 1:779:A:GLY:H    | 10       | 0.11          |
| (1,1490) | 1:776:A:ILE:HG21 | 1:777:A:SER:H    | 20       | 0.11          |
| (1,1490) | 1:776:A:ILE:HG22 | 1:777:A:SER:H    | 20       | 0.11          |
| (1,1490) | 1:776:A:ILE:HG23 | 1:777:A:SER:H    | 20       | 0.11          |
| (1,1486) | 1:775:A:LEU:HD11 | 1:776:A:ILE:H    | 17       | 0.11          |
| (1,1486) | 1:775:A:LEU:HD12 | 1:776:A:ILE:H    | 17       | 0.11          |
| (1,1486) | 1:775:A:LEU:HD13 | 1:776:A:ILE:H    | 17       | 0.11          |
| (1,1486) | 1:775:A:LEU:HD11 | 1:776:A:ILE:H    | 20       | 0.11          |
| (1,1486) | 1:775:A:LEU:HD12 | 1:776:A:ILE:H    | 20       | 0.11          |
| (1,1486) | 1:775:A:LEU:HD13 | 1:776:A:ILE:H    | 20       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 6        | 0.11          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 6        | 0.11          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 6        | 0.11          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 7        | 0.11          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 7        | 0.11          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 7        | 0.11          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 14       | 0.11          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 14       | 0.11          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 14       | 0.11          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD11 | 17       | 0.11          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD12 | 17       | 0.11          |
| (1,1448) | 1:773:A:ALA:H    | 1:775:A:LEU:HD13 | 17       | 0.11          |
| (1,1149) | 1:743:A:ILE:HG21 | 1:747:A:GLN:HE22 | 14       | 0.11          |
| (1,1149) | 1:743:A:ILE:HG22 | 1:747:A:GLN:HE22 | 14       | 0.11          |
| (1,1149) | 1:743:A:ILE:HG23 | 1:747:A:GLN:HE22 | 14       | 0.11          |
| (1,1120) | 1:743:A:ILE:HD11 | 1:744:A:SER:H    | 6        | 0.11          |
| (1,1120) | 1:743:A:ILE:HD12 | 1:744:A:SER:H    | 6        | 0.11          |
| (1,1120) | 1:743:A:ILE:HD13 | 1:744:A:SER:H    | 6        | 0.11          |
| (1,1120) | 1:743:A:ILE:HD11 | 1:744:A:SER:H    | 12       | 0.11          |
| (1,1120) | 1:743:A:ILE:HD12 | 1:744:A:SER:H    | 12       | 0.11          |
| (1,1120) | 1:743:A:ILE:HD13 | 1:744:A:SER:H    | 12       | 0.11          |
| (1,1120) | 1:743:A:ILE:HD11 | 1:744:A:SER:H    | 19       | 0.11          |
| (1,1120) | 1:743:A:ILE:HD12 | 1:744:A:SER:H    | 19       | 0.11          |
| (1,1120) | 1:743:A:ILE:HD13 | 1:744:A:SER:H    | 19       | 0.11          |
| (1,874)  | 1:751:A:PHE:HE2  | 1:813:A:ILE:HD11 | 3        | 0.11          |
| (1,874)  | 1:751:A:PHE:HE2  | 1:813:A:ILE:HD12 | 3        | 0.11          |
| (1,874)  | 1:751:A:PHE:HE2  | 1:813:A:ILE:HD13 | 3        | 0.11          |
| (1,844)  | 1:829:A:VAL:HG21 | 1:830:A:MET:HB2  | 11       | 0.11          |
| (1,844)  | 1:829:A:VAL:HG22 | 1:830:A:MET:HB2  | 11       | 0.11          |
| (1,844)  | 1:829:A:VAL:HG23 | 1:830:A:MET:HB2  | 11       | 0.11          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 2        | 0.11          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 2        | 0.11          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 2        | 0.11          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD21 | 2        | 0.11          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD22 | 2        | 0.11          |
| (1,804)  | 1:845:A:MET:HE2  | 1:877:A:LEU:HD23 | 2        | 0.11          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD21 | 2        | 0.11          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD22 | 2        | 0.11          |
| (1,804)  | 1:845:A:MET:HE3  | 1:877:A:LEU:HD23 | 2        | 0.11          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD21 | 5        | 0.11          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD22 | 5        | 0.11          |
| (1,804)  | 1:845:A:MET:HE1  | 1:877:A:LEU:HD23 | 5        | 0.11          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,804) | 1:845:A:MET:HE2 | 1:877:A:LEU:HD21 | 5        | 0.11          |
| (1,804) | 1:845:A:MET:HE2 | 1:877:A:LEU:HD22 | 5        | 0.11          |
| (1,804) | 1:845:A:MET:HE2 | 1:877:A:LEU:HD23 | 5        | 0.11          |
| (1,804) | 1:845:A:MET:HE3 | 1:877:A:LEU:HD21 | 5        | 0.11          |
| (1,804) | 1:845:A:MET:HE3 | 1:877:A:LEU:HD22 | 5        | 0.11          |
| (1,804) | 1:845:A:MET:HE3 | 1:877:A:LEU:HD23 | 5        | 0.11          |
| (1,804) | 1:845:A:MET:HE1 | 1:877:A:LEU:HD21 | 8        | 0.11          |
| (1,804) | 1:845:A:MET:HE1 | 1:877:A:LEU:HD22 | 8        | 0.11          |
| (1,804) | 1:845:A:MET:HE1 | 1:877:A:LEU:HD23 | 8        | 0.11          |
| (1,804) | 1:845:A:MET:HE2 | 1:877:A:LEU:HD21 | 8        | 0.11          |
| (1,804) | 1:845:A:MET:HE2 | 1:877:A:LEU:HD22 | 8        | 0.11          |
| (1,804) | 1:845:A:MET:HE2 | 1:877:A:LEU:HD23 | 8        | 0.11          |
| (1,804) | 1:845:A:MET:HE3 | 1:877:A:LEU:HD21 | 8        | 0.11          |
| (1,804) | 1:845:A:MET:HE3 | 1:877:A:LEU:HD22 | 8        | 0.11          |
| (1,804) | 1:845:A:MET:HE3 | 1:877:A:LEU:HD23 | 8        | 0.11          |
| (1,804) | 1:845:A:MET:HE1 | 1:877:A:LEU:HD21 | 16       | 0.11          |
| (1,804) | 1:845:A:MET:HE1 | 1:877:A:LEU:HD22 | 16       | 0.11          |
| (1,804) | 1:845:A:MET:HE1 | 1:877:A:LEU:HD23 | 16       | 0.11          |
| (1,804) | 1:845:A:MET:HE2 | 1:877:A:LEU:HD21 | 16       | 0.11          |
| (1,804) | 1:845:A:MET:HE2 | 1:877:A:LEU:HD22 | 16       | 0.11          |
| (1,804) | 1:845:A:MET:HE2 | 1:877:A:LEU:HD23 | 16       | 0.11          |
| (1,804) | 1:845:A:MET:HE3 | 1:877:A:LEU:HD21 | 16       | 0.11          |
| (1,804) | 1:845:A:MET:HE3 | 1:877:A:LEU:HD22 | 16       | 0.11          |
| (1,804) | 1:845:A:MET:HE3 | 1:877:A:LEU:HD23 | 16       | 0.11          |
| (1,534) | 1:819:A:GLU:HA  | 1:821:A:ALA:HB1  | 13       | 0.11          |
| (1,534) | 1:819:A:GLU:HA  | 1:821:A:ALA:HB2  | 13       | 0.11          |
| (1,534) | 1:819:A:GLU:HA  | 1:821:A:ALA:HB3  | 13       | 0.11          |
| (1,381) | 1:795:A:ILE:HA  | 1:798:A:ILE:HG21 | 13       | 0.11          |
| (1,381) | 1:795:A:ILE:HA  | 1:798:A:ILE:HG22 | 13       | 0.11          |
| (1,381) | 1:795:A:ILE:HA  | 1:798:A:ILE:HG23 | 13       | 0.11          |
| (1,307) | 1:785:A:ASP:HB3 | 1:787:A:GLN:H    | 2        | 0.11          |
| (1,251) | 1:773:A:ALA:HA  | 1:776:A:ILE:HG21 | 5        | 0.11          |
| (1,251) | 1:773:A:ALA:HA  | 1:776:A:ILE:HG22 | 5        | 0.11          |
| (1,251) | 1:773:A:ALA:HA  | 1:776:A:ILE:HG23 | 5        | 0.11          |
| (1,228) | 1:771:A:PHE:HA  | 1:775:A:LEU:HD21 | 11       | 0.11          |
| (1,228) | 1:771:A:PHE:HA  | 1:775:A:LEU:HD22 | 11       | 0.11          |
| (1,228) | 1:771:A:PHE:HA  | 1:775:A:LEU:HD23 | 11       | 0.11          |
| (1,228) | 1:771:A:PHE:HA  | 1:775:A:LEU:HD21 | 14       | 0.11          |
| (1,228) | 1:771:A:PHE:HA  | 1:775:A:LEU:HD22 | 14       | 0.11          |
| (1,228) | 1:771:A:PHE:HA  | 1:775:A:LEU:HD23 | 14       | 0.11          |
| (1,214) | 1:773:A:ALA:HA  | 1:775:A:LEU:HD11 | 13       | 0.11          |
| (1,214) | 1:773:A:ALA:HA  | 1:775:A:LEU:HD12 | 13       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,214)  | 1:773:A:ALA:HA   | 1:775:A:LEU:HD13 | 13       | 0.11          |
| (1,116)  | 1:765:A:THR:HG21 | 1:771:A:PHE:HZ   | 4        | 0.11          |
| (1,116)  | 1:765:A:THR:HG22 | 1:771:A:PHE:HZ   | 4        | 0.11          |
| (1,116)  | 1:765:A:THR:HG23 | 1:771:A:PHE:HZ   | 4        | 0.11          |
| (1,116)  | 1:765:A:THR:HG21 | 1:771:A:PHE:HZ   | 11       | 0.11          |
| (1,116)  | 1:765:A:THR:HG22 | 1:771:A:PHE:HZ   | 11       | 0.11          |
| (1,116)  | 1:765:A:THR:HG23 | 1:771:A:PHE:HZ   | 11       | 0.11          |
| (1,116)  | 1:765:A:THR:HG21 | 1:771:A:PHE:HZ   | 18       | 0.11          |
| (1,116)  | 1:765:A:THR:HG22 | 1:771:A:PHE:HZ   | 18       | 0.11          |
| (1,116)  | 1:765:A:THR:HG23 | 1:771:A:PHE:HZ   | 18       | 0.11          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE1  | 19       | 0.11          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE2  | 19       | 0.11          |
| (1,46)   | 1:748:A:MET:HA   | 1:748:A:MET:HE3  | 19       | 0.11          |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 15       | 0.1           |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 15       | 0.1           |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 15       | 0.1           |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 15       | 0.1           |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 15       | 0.1           |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 15       | 0.1           |
| (1,2634) | 1:829:A:VAL:HG11 | 1:831:A:ALA:H    | 20       | 0.1           |
| (1,2634) | 1:829:A:VAL:HG12 | 1:831:A:ALA:H    | 20       | 0.1           |
| (1,2634) | 1:829:A:VAL:HG13 | 1:831:A:ALA:H    | 20       | 0.1           |
| (1,2634) | 1:829:A:VAL:HG21 | 1:831:A:ALA:H    | 20       | 0.1           |
| (1,2634) | 1:829:A:VAL:HG22 | 1:831:A:ALA:H    | 20       | 0.1           |
| (1,2634) | 1:829:A:VAL:HG23 | 1:831:A:ALA:H    | 20       | 0.1           |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG11 | 15       | 0.1           |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG12 | 15       | 0.1           |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG13 | 15       | 0.1           |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG21 | 15       | 0.1           |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG22 | 15       | 0.1           |
| (1,2628) | 1:828:A:GLN:HE22 | 1:829:A:VAL:HG23 | 15       | 0.1           |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG11 | 15       | 0.1           |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG12 | 15       | 0.1           |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG13 | 15       | 0.1           |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG21 | 15       | 0.1           |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG22 | 15       | 0.1           |
| (1,2627) | 1:828:A:GLN:HE21 | 1:829:A:VAL:HG23 | 15       | 0.1           |
| (1,2621) | 1:824:A:ASP:HB2  | 1:826:A:ALA:H    | 20       | 0.1           |
| (1,2621) | 1:824:A:ASP:HB3  | 1:826:A:ALA:H    | 20       | 0.1           |
| (1,2380) | 1:872:A:SER:H    | 1:873:A:VAL:HG21 | 17       | 0.1           |
| (1,2380) | 1:872:A:SER:H    | 1:873:A:VAL:HG22 | 17       | 0.1           |
| (1,2380) | 1:872:A:SER:H    | 1:873:A:VAL:HG23 | 17       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2359) | 1:843:A:ILE:HG21 | 1:865:A:ALA:H    | 16       | 0.1           |
| (1,2359) | 1:843:A:ILE:HG22 | 1:865:A:ALA:H    | 16       | 0.1           |
| (1,2359) | 1:843:A:ILE:HG23 | 1:865:A:ALA:H    | 16       | 0.1           |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 1        | 0.1           |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 1        | 0.1           |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 1        | 0.1           |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD11 | 7        | 0.1           |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD12 | 7        | 0.1           |
| (1,2302) | 1:860:A:CYS:H    | 1:861:A:ILE:HD13 | 7        | 0.1           |
| (1,2236) | 1:852:A:LEU:HD11 | 1:856:A:GLN:H    | 4        | 0.1           |
| (1,2236) | 1:852:A:LEU:HD12 | 1:856:A:GLN:H    | 4        | 0.1           |
| (1,2236) | 1:852:A:LEU:HD13 | 1:856:A:GLN:H    | 4        | 0.1           |
| (1,2143) | 1:843:A:ILE:HD11 | 1:844:A:THR:H    | 3        | 0.1           |
| (1,2143) | 1:843:A:ILE:HD12 | 1:844:A:THR:H    | 3        | 0.1           |
| (1,2143) | 1:843:A:ILE:HD13 | 1:844:A:THR:H    | 3        | 0.1           |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD11 | 12       | 0.1           |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD12 | 12       | 0.1           |
| (1,2088) | 1:840:A:LYS:H    | 1:843:A:ILE:HD13 | 12       | 0.1           |
| (1,2063) | 1:835:A:ILE:H    | 1:837:A:ALA:H    | 9        | 0.1           |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB1  | 1        | 0.1           |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB2  | 1        | 0.1           |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB3  | 1        | 0.1           |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB1  | 7        | 0.1           |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB2  | 7        | 0.1           |
| (1,2058) | 1:836:A:LEU:H    | 1:837:A:ALA:HB3  | 7        | 0.1           |
| (1,2038) | 1:836:A:LEU:HD11 | 1:848:A:LEU:H    | 5        | 0.1           |
| (1,2038) | 1:836:A:LEU:HD12 | 1:848:A:LEU:H    | 5        | 0.1           |
| (1,2038) | 1:836:A:LEU:HD13 | 1:848:A:LEU:H    | 5        | 0.1           |
| (1,1945) | 1:743:A:ILE:HD11 | 1:749:A:ASN:H    | 10       | 0.1           |
| (1,1945) | 1:743:A:ILE:HD12 | 1:749:A:ASN:H    | 10       | 0.1           |
| (1,1945) | 1:743:A:ILE:HD13 | 1:749:A:ASN:H    | 10       | 0.1           |
| (1,1893) | 1:799:A:VAL:HG11 | 1:811:A:ALA:H    | 3        | 0.1           |
| (1,1893) | 1:799:A:VAL:HG12 | 1:811:A:ALA:H    | 3        | 0.1           |
| (1,1893) | 1:799:A:VAL:HG13 | 1:811:A:ALA:H    | 3        | 0.1           |
| (1,1742) | 1:802:A:ASN:H    | 1:804:A:LEU:HD21 | 3        | 0.1           |
| (1,1742) | 1:802:A:ASN:H    | 1:804:A:LEU:HD22 | 3        | 0.1           |
| (1,1742) | 1:802:A:ASN:H    | 1:804:A:LEU:HD23 | 3        | 0.1           |
| (1,1709) | 1:795:A:ILE:HG21 | 1:798:A:ILE:H    | 1        | 0.1           |
| (1,1709) | 1:795:A:ILE:HG22 | 1:798:A:ILE:H    | 1        | 0.1           |
| (1,1709) | 1:795:A:ILE:HG23 | 1:798:A:ILE:H    | 1        | 0.1           |
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG21 | 11       | 0.1           |
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG22 | 11       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1666) | 1:794:A:ARG:H    | 1:795:A:ILE:HG23 | 11       | 0.1           |
| (1,1595) | 1:782:A:ILE:HG21 | 1:788:A:GLY:H    | 7        | 0.1           |
| (1,1595) | 1:782:A:ILE:HG22 | 1:788:A:GLY:H    | 7        | 0.1           |
| (1,1595) | 1:782:A:ILE:HG23 | 1:788:A:GLY:H    | 7        | 0.1           |
| (1,1543) | 1:776:A:ILE:HD11 | 1:782:A:ILE:H    | 7        | 0.1           |
| (1,1543) | 1:776:A:ILE:HD12 | 1:782:A:ILE:H    | 7        | 0.1           |
| (1,1543) | 1:776:A:ILE:HD13 | 1:782:A:ILE:H    | 7        | 0.1           |
| (1,1526) | 1:776:A:ILE:HG21 | 1:780:A:TYR:H    | 10       | 0.1           |
| (1,1526) | 1:776:A:ILE:HG22 | 1:780:A:TYR:H    | 10       | 0.1           |
| (1,1526) | 1:776:A:ILE:HG23 | 1:780:A:TYR:H    | 10       | 0.1           |
| (1,1526) | 1:776:A:ILE:HG21 | 1:780:A:TYR:H    | 13       | 0.1           |
| (1,1526) | 1:776:A:ILE:HG22 | 1:780:A:TYR:H    | 13       | 0.1           |
| (1,1526) | 1:776:A:ILE:HG23 | 1:780:A:TYR:H    | 13       | 0.1           |
| (1,1490) | 1:776:A:ILE:HG21 | 1:777:A:SER:H    | 3        | 0.1           |
| (1,1490) | 1:776:A:ILE:HG22 | 1:777:A:SER:H    | 3        | 0.1           |
| (1,1490) | 1:776:A:ILE:HG23 | 1:777:A:SER:H    | 3        | 0.1           |
| (1,1490) | 1:776:A:ILE:HG21 | 1:777:A:SER:H    | 6        | 0.1           |
| (1,1490) | 1:776:A:ILE:HG22 | 1:777:A:SER:H    | 6        | 0.1           |
| (1,1490) | 1:776:A:ILE:HG23 | 1:777:A:SER:H    | 6        | 0.1           |
| (1,1486) | 1:775:A:LEU:HD11 | 1:776:A:ILE:H    | 3        | 0.1           |
| (1,1486) | 1:775:A:LEU:HD12 | 1:776:A:ILE:H    | 3        | 0.1           |
| (1,1486) | 1:775:A:LEU:HD13 | 1:776:A:ILE:H    | 3        | 0.1           |
| (1,1420) | 1:771:A:PHE:H    | 1:772:A:LYS:HB2  | 13       | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 3        | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 3        | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 3        | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 8        | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 8        | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 8        | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 17       | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 17       | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 17       | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD11 | 18       | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD12 | 18       | 0.1           |
| (1,1332) | 1:761:A:ASP:H    | 1:766:A:LEU:HD13 | 18       | 0.1           |
| (1,1149) | 1:743:A:ILE:HG21 | 1:747:A:GLN:HE22 | 4        | 0.1           |
| (1,1149) | 1:743:A:ILE:HG22 | 1:747:A:GLN:HE22 | 4        | 0.1           |
| (1,1149) | 1:743:A:ILE:HG23 | 1:747:A:GLN:HE22 | 4        | 0.1           |
| (1,1031) | 1:842:A:TYR:HD1  | 1:867:A:TYR:HD2  | 5        | 0.1           |
| (1,976)  | 1:752:A:ARG:HD2  | 1:809:A:PHE:HZ   | 13       | 0.1           |
| (1,764)  | 1:865:A:ALA:HB1  | 1:882:A:PHE:HB2  | 3        | 0.1           |
| (1,764)  | 1:865:A:ALA:HB2  | 1:882:A:PHE:HB2  | 3        | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,764) | 1:865:A:ALA:HB3  | 1:882:A:PHE:HB2  | 3        | 0.1           |
| (1,727) | 1:782:A:ILE:HD11 | 1:791:A:GLU:HB2  | 10       | 0.1           |
| (1,727) | 1:782:A:ILE:HD12 | 1:791:A:GLU:HB2  | 10       | 0.1           |
| (1,727) | 1:782:A:ILE:HD13 | 1:791:A:GLU:HB2  | 10       | 0.1           |
| (1,727) | 1:782:A:ILE:HD11 | 1:791:A:GLU:HB2  | 17       | 0.1           |
| (1,727) | 1:782:A:ILE:HD12 | 1:791:A:GLU:HB2  | 17       | 0.1           |
| (1,727) | 1:782:A:ILE:HD13 | 1:791:A:GLU:HB2  | 17       | 0.1           |
| (1,599) | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD11 | 19       | 0.1           |
| (1,599) | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD12 | 19       | 0.1           |
| (1,599) | 1:836:A:LEU:HB2  | 1:843:A:ILE:HD13 | 19       | 0.1           |
| (1,409) | 1:802:A:ASN:HB3  | 1:804:A:LEU:HG   | 16       | 0.1           |
| (1,402) | 1:800:A:ASP:HA   | 1:804:A:LEU:HB2  | 13       | 0.1           |
| (1,251) | 1:773:A:ALA:HA   | 1:776:A:ILE:HG21 | 7        | 0.1           |
| (1,251) | 1:773:A:ALA:HA   | 1:776:A:ILE:HG22 | 7        | 0.1           |
| (1,251) | 1:773:A:ALA:HA   | 1:776:A:ILE:HG23 | 7        | 0.1           |
| (1,228) | 1:771:A:PHE:HA   | 1:775:A:LEU:HD21 | 20       | 0.1           |
| (1,228) | 1:771:A:PHE:HA   | 1:775:A:LEU:HD22 | 20       | 0.1           |
| (1,228) | 1:771:A:PHE:HA   | 1:775:A:LEU:HD23 | 20       | 0.1           |
| (1,97)  | 1:785:A:ASP:HB2  | 1:786:A:PRO:HD2  | 1        | 0.1           |
| (1,12)  | 1:798:A:ILE:HG21 | 1:800:A:ASP:H    | 17       | 0.1           |
| (1,12)  | 1:798:A:ILE:HG22 | 1:800:A:ASP:H    | 17       | 0.1           |
| (1,12)  | 1:798:A:ILE:HG23 | 1:800:A:ASP:H    | 17       | 0.1           |

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

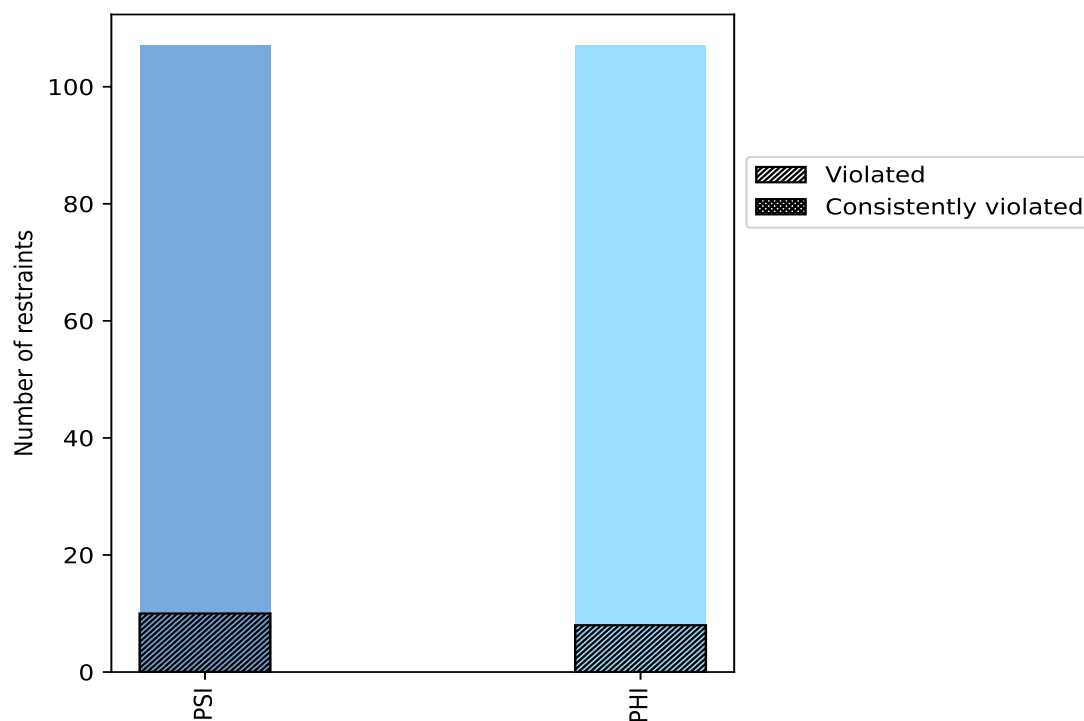
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 107   | 50.0           | 10                    | 9.3            | 4.7            | 0                                  | 0.0            | 0.0            |
| PHI        | 107   | 50.0           | 8                     | 7.5            | 3.7            | 0                                  | 0.0            | 0.0            |
| Total      | 214   | 100.0          | 18                    | 8.4            | 8.4            | 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](#)



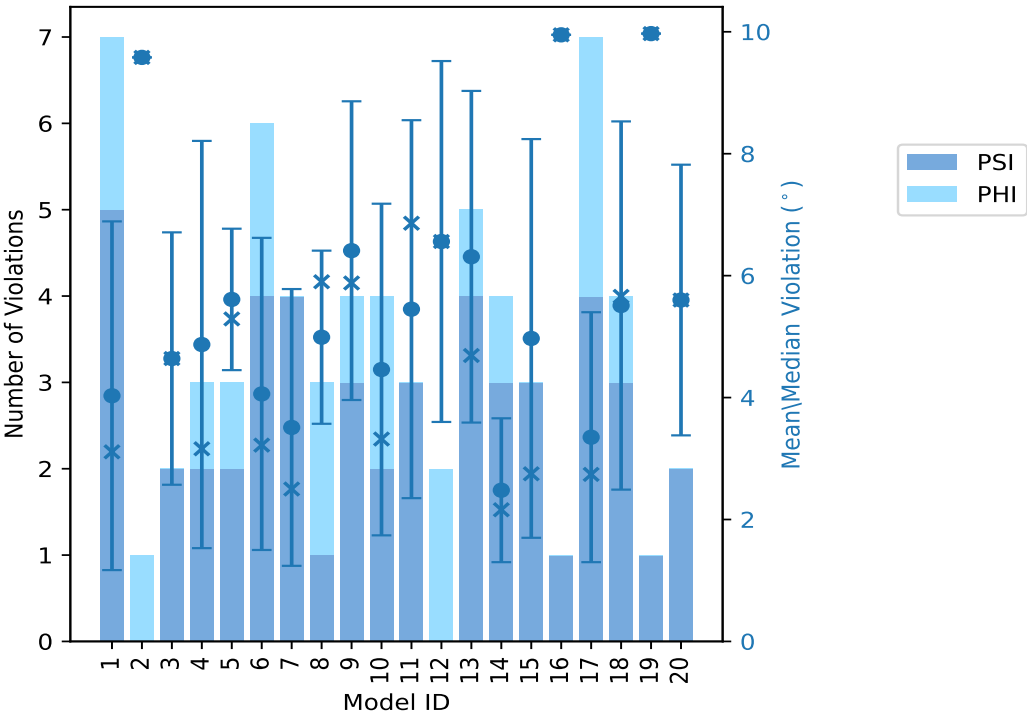
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 5                    | 2   | 7     | 4.03     | 9.84    | 2.86   | 3.11       |
| 2        | 0                    | 1   | 1     | 9.58     | 9.58    | 0.0    | 9.58       |
| 3        | 2                    | 0   | 2     | 4.64     | 6.71    | 2.07   | 4.64       |
| 4        | 2                    | 1   | 3     | 4.87     | 9.54    | 3.34   | 3.16       |
| 5        | 2                    | 1   | 3     | 5.61     | 7.17    | 1.16   | 5.29       |
| 6        | 4                    | 2   | 6     | 4.06     | 9.0     | 2.56   | 3.22       |
| 7        | 4                    | 0   | 4     | 3.51     | 7.38    | 2.27   | 2.5        |
| 8        | 1                    | 2   | 3     | 4.99     | 6.08    | 1.42   | 5.9        |
| 9        | 3                    | 1   | 4     | 6.41     | 9.86    | 2.45   | 5.88       |
| 10       | 2                    | 2   | 4     | 4.46     | 9.01    | 2.72   | 3.32       |
| 11       | 3                    | 0   | 3     | 5.45     | 8.34    | 3.1    | 6.86       |
| 12       | 0                    | 2   | 2     | 6.56     | 9.52    | 2.96   | 6.56       |
| 13       | 4                    | 1   | 5     | 6.31     | 9.89    | 2.72   | 4.69       |
| 14       | 3                    | 1   | 4     | 2.48     | 4.31    | 1.18   | 2.16       |
| 15       | 3                    | 0   | 3     | 4.97     | 9.59    | 3.27   | 2.75       |
| 16       | 1                    | 0   | 1     | 9.95     | 9.95    | 0.0    | 9.95       |
| 17       | 4                    | 3   | 7     | 3.35     | 7.96    | 2.05   | 2.74       |
| 18       | 3                    | 1   | 4     | 5.51     | 9.01    | 3.02   | 5.66       |
| 19       | 1                    | 0   | 1     | 9.97     | 9.97    | 0.0    | 9.97       |
| 20       | 2                    | 0   | 2     | 5.6      | 7.81    | 2.22   | 5.6        |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

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

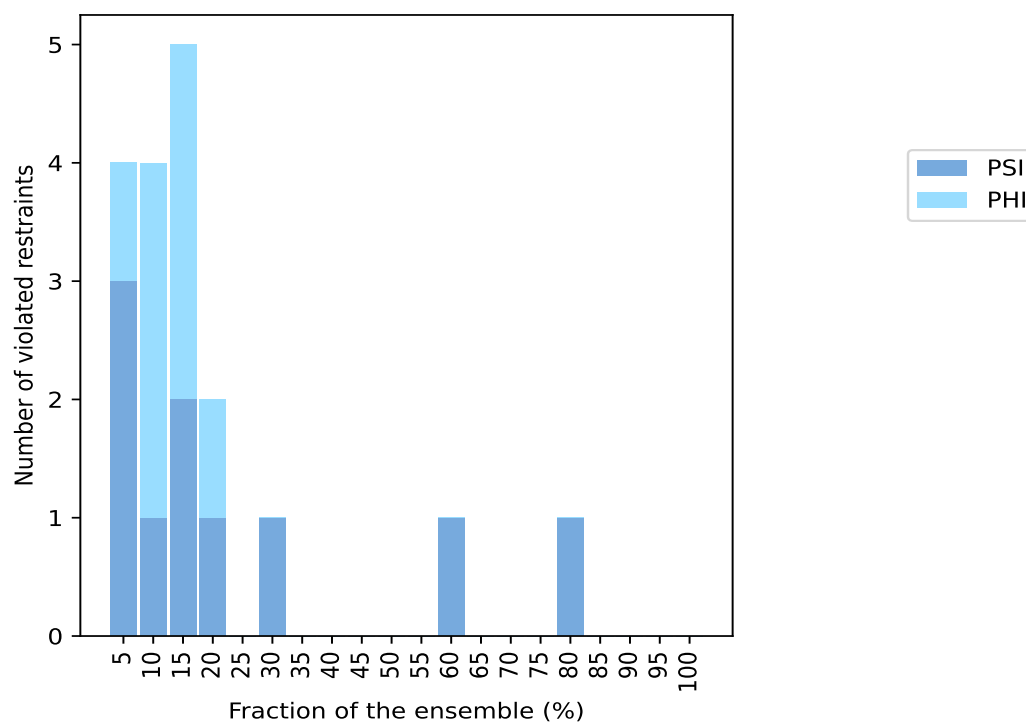
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 1                             | 0   | 1     | 12                       | 60.0  |
| 0                             | 0   | 0     | 13                       | 65.0  |
| 0                             | 0   | 0     | 14                       | 70.0  |
| 0                             | 0   | 0     | 15                       | 75.0  |
| 1                             | 0   | 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](#)



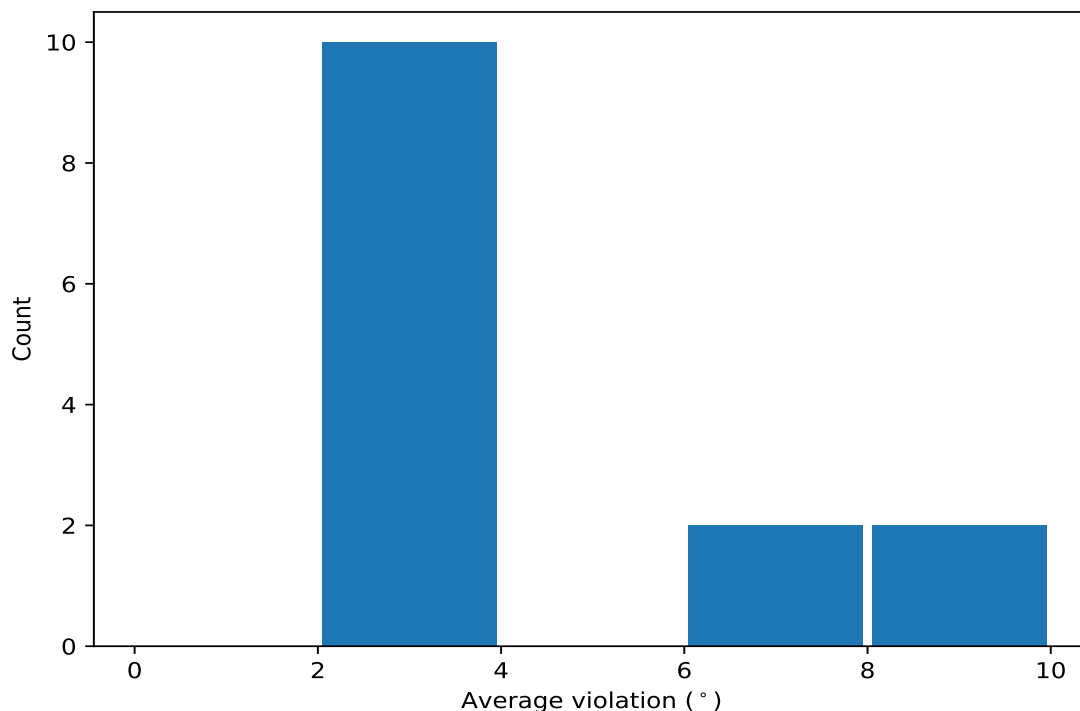
## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 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.

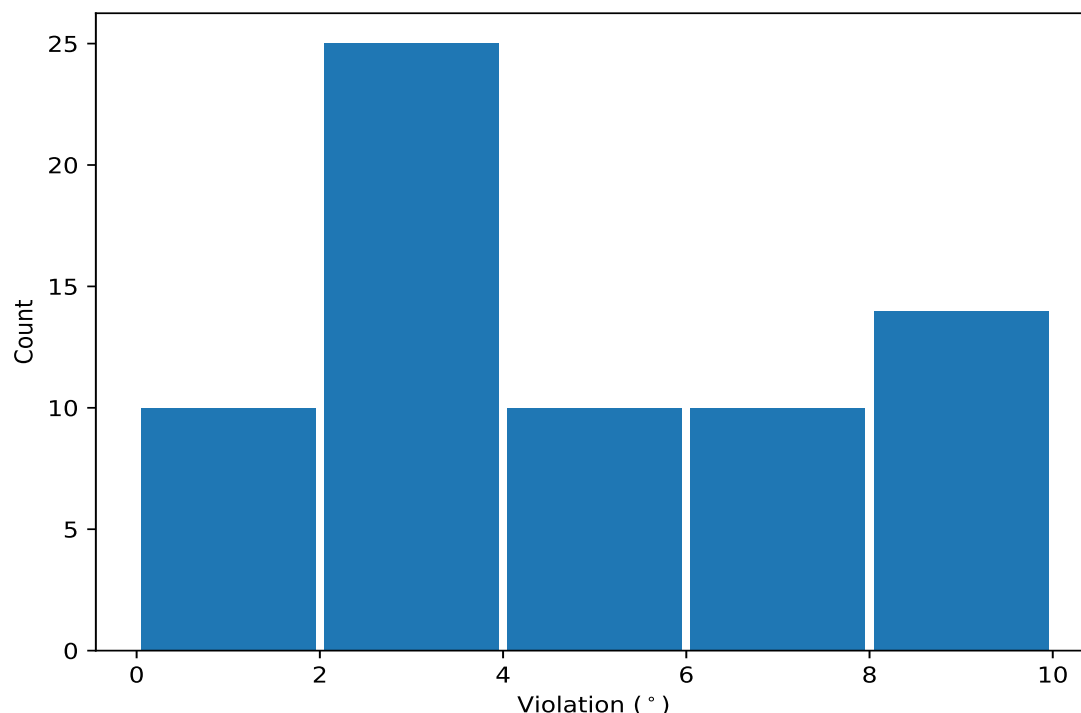
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 16                  | 7.23 | 2.07            | 7.49   |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 12                  | 2.65 | 0.95            | 2.56   |
| (1,172) | 1:848:A:LEU:N | 1:848:A:LEU:CA | 1:848:A:LEU:C  | 1:849:A:ARG:N | 6                   | 3.78 | 2.69            | 2.96   |
| (1,130) | 1:820:A:THR:N | 1:820:A:THR:CA | 1:820:A:THR:C  | 1:821:A:ALA:N | 4                   | 9.84 | 0.15            | 9.9    |
| (1,151) | 1:835:A:ILE:C | 1:836:A:LEU:N  | 1:836:A:LEU:CA | 1:836:A:LEU:C | 4                   | 2.31 | 0.87            | 2.37   |
| (1,131) | 1:825:A:THR:C | 1:826:A:ALA:N  | 1:826:A:ALA:CA | 1:826:A:ALA:C | 3                   | 9.37 | 0.26            | 9.52   |
| (1,213) | 1:883:A:SER:C | 1:884:A:THR:N  | 1:884:A:THR:CA | 1:884:A:THR:C | 3                   | 6.64 | 0.97            | 6.58   |
| (1,125) | 1:817:A:SER:C | 1:818:A:ARG:N  | 1:818:A:ARG:CA | 1:818:A:ARG:C | 3                   | 3.56 | 1.71            | 4.15   |
| (1,36)  | 1:761:A:ASP:N | 1:761:A:ASP:CA | 1:761:A:ASP:C  | 1:762:A:HIS:N | 3                   | 3.5  | 0.85            | 3.11   |
| (1,182) | 1:855:A:ASP:N | 1:855:A:ASP:CA | 1:855:A:ASP:C  | 1:856:A:GLN:N | 3                   | 3.01 | 0.58            | 3.31   |
| (1,120) | 1:815:A:PHE:N | 1:815:A:PHE:CA | 1:815:A:PHE:C  | 1:816:A:MET:N | 2                   | 3.16 | 0.36            | 3.16   |
| (1,1)   | 1:743:A:ILE:C | 1:744:A:SER:N  | 1:744:A:SER:CA | 1:744:A:SER:C | 2                   | 3.06 | 0.52            | 3.06   |
| (1,105) | 1:807:A:VAL:C | 1:808:A:THR:N  | 1:808:A:THR:CA | 1:808:A:THR:C | 2                   | 2.39 | 0.78            | 2.39   |
| (1,83)  | 1:793:A:ALA:C | 1:794:A:ARG:N  | 1:794:A:ARG:CA | 1:794:A:ARG:C | 2                   | 2.35 | 0.63            | 2.35   |

<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 (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,130) | 1:820:A:THR:N | 1:820:A:THR:CA | 1:820:A:THR:C  | 1:821:A:ALA:N | 19       | 9.97          |
| (1,130) | 1:820:A:THR:N | 1:820:A:THR:CA | 1:820:A:THR:C  | 1:821:A:ALA:N | 16       | 9.95          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 13       | 9.89          |
| (1,130) | 1:820:A:THR:N | 1:820:A:THR:CA | 1:820:A:THR:C  | 1:821:A:ALA:N | 9        | 9.86          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 1        | 9.84          |
| (1,130) | 1:820:A:THR:N | 1:820:A:THR:CA | 1:820:A:THR:C  | 1:821:A:ALA:N | 15       | 9.59          |
| (1,131) | 1:825:A:THR:C | 1:826:A:ALA:N  | 1:826:A:ALA:CA | 1:826:A:ALA:C | 2        | 9.58          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 4        | 9.54          |
| (1,131) | 1:825:A:THR:C | 1:826:A:ALA:N  | 1:826:A:ALA:CA | 1:826:A:ALA:C | 12       | 9.52          |
| (1,172) | 1:848:A:LEU:N | 1:848:A:LEU:CA | 1:848:A:LEU:C  | 1:849:A:ARG:N | 13       | 9.3           |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 18       | 9.01          |
| (1,131) | 1:825:A:THR:C | 1:826:A:ALA:N  | 1:826:A:ALA:CA | 1:826:A:ALA:C | 10       | 9.01          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 6        | 9.0           |
| (1,132) | 1:826:A:ALA:N | 1:826:A:ALA:CA | 1:826:A:ALA:C  | 1:827:A:ASP:N | 11       | 8.34          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 17       | 7.96          |
| (1,213) | 1:883:A:SER:C | 1:884:A:THR:N  | 1:884:A:THR:CA | 1:884:A:THR:C | 18       | 7.86          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 20       | 7.81          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 9        | 7.6           |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 7        | 7.38          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 5        | 7.17          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 11       | 6.86          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 3        | 6.71          |
| (1,213) | 1:883:A:SER:C | 1:884:A:THR:N  | 1:884:A:THR:CA | 1:884:A:THR:C | 1        | 6.58          |
| (1,127) | 1:818:A:ARG:C | 1:819:A:GLU:N  | 1:819:A:GLU:CA | 1:819:A:GLU:C | 8        | 6.08          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 8        | 5.9           |
| (1,213) | 1:883:A:SER:C | 1:884:A:THR:N  | 1:884:A:THR:CA | 1:884:A:THR:C | 6        | 5.49          |
| (1,125) | 1:817:A:SER:C | 1:818:A:ARG:N  | 1:818:A:ARG:CA | 1:818:A:ARG:C | 5        | 5.29          |
| (1,36)  | 1:761:A:ASP:N | 1:761:A:ASP:CA | 1:761:A:ASP:C  | 1:762:A:HIS:N | 13       | 4.69          |
| (1,172) | 1:848:A:LEU:N | 1:848:A:LEU:CA | 1:848:A:LEU:C  | 1:849:A:ARG:N | 5        | 4.38          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 14       | 4.31          |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 13       | 4.26          |
| (1,125) | 1:817:A:SER:C | 1:818:A:ARG:N  | 1:818:A:ARG:CA | 1:818:A:ARG:C | 9        | 4.15          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 10       | 4.1           |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 9        | 4.03          |
| (1,172) | 1:848:A:LEU:N | 1:848:A:LEU:CA | 1:848:A:LEU:C  | 1:849:A:ARG:N | 17       | 3.69          |
| (1,1)   | 1:743:A:ILE:C | 1:744:A:SER:N  | 1:744:A:SER:CA | 1:744:A:SER:C | 12       | 3.59          |
| (1,182) | 1:855:A:ASP:N | 1:855:A:ASP:CA | 1:855:A:ASP:C  | 1:856:A:GLN:N | 6        | 3.52          |
| (1,120) | 1:815:A:PHE:N | 1:815:A:PHE:CA | 1:815:A:PHE:C  | 1:816:A:MET:N | 17       | 3.52          |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 18       | 3.46          |
| (1,151) | 1:835:A:ILE:C | 1:836:A:LEU:N  | 1:836:A:LEU:CA | 1:836:A:LEU:C | 13       | 3.42          |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 20       | 3.38          |
| (1,182) | 1:855:A:ASP:N | 1:855:A:ASP:CA | 1:855:A:ASP:C  | 1:856:A:GLN:N | 1        | 3.31          |
| (1,105) | 1:807:A:VAL:C | 1:808:A:THR:N  | 1:808:A:THR:CA | 1:808:A:THR:C | 4        | 3.16          |
| (1,36)  | 1:761:A:ASP:N | 1:761:A:ASP:CA | 1:761:A:ASP:C  | 1:762:A:HIS:N | 1        | 3.11          |
| (1,83)  | 1:793:A:ALA:C | 1:794:A:ARG:N  | 1:794:A:ARG:CA | 1:794:A:ARG:C | 8        | 2.98          |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 6        | 2.92          |
| (1,120) | 1:815:A:PHE:N | 1:815:A:PHE:CA | 1:815:A:PHE:C  | 1:816:A:MET:N | 7        | 2.8           |
| (1,78)  | 1:791:A:GLU:N | 1:791:A:GLU:CA | 1:791:A:GLU:C  | 1:792:A:PHE:N | 15       | 2.75          |
| (1,151) | 1:835:A:ILE:C | 1:836:A:LEU:N  | 1:836:A:LEU:CA | 1:836:A:LEU:C | 17       | 2.74          |
| (1,36)  | 1:761:A:ASP:N | 1:761:A:ASP:CA | 1:761:A:ASP:C  | 1:762:A:HIS:N | 14       | 2.71          |
| (1,208) | 1:878:A:ASP:N | 1:878:A:ASP:CA | 1:878:A:ASP:C  | 1:879:A:TYR:N | 15       | 2.58          |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 3        | 2.57          |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 17       | 2.56          |
| (1,1)   | 1:743:A:ILE:C | 1:744:A:SER:N  | 1:744:A:SER:CA | 1:744:A:SER:C | 10       | 2.54          |
| (1,172) | 1:848:A:LEU:N | 1:848:A:LEU:CA | 1:848:A:LEU:C  | 1:849:A:ARG:N | 1        | 2.23          |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 7        | 2.2           |
| (1,182) | 1:855:A:ASP:N | 1:855:A:ASP:CA | 1:855:A:ASP:C  | 1:856:A:GLN:N | 10       | 2.19          |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 1        | 2.08          |
| (1,151) | 1:835:A:ILE:C | 1:836:A:LEU:N  | 1:836:A:LEU:CA | 1:836:A:LEU:C | 6        | 2.0           |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 4        | 1.91          |
| (1,83)  | 1:793:A:ALA:C | 1:794:A:ARG:N  | 1:794:A:ARG:CA | 1:794:A:ARG:C | 17       | 1.72          |
| (1,128) | 1:819:A:GLU:N | 1:819:A:GLU:CA | 1:819:A:GLU:C  | 1:820:A:THR:N | 18       | 1.7           |
| (1,172) | 1:848:A:LEU:N | 1:848:A:LEU:CA | 1:848:A:LEU:C  | 1:849:A:ARG:N | 7        | 1.67          |
| (1,105) | 1:807:A:VAL:C | 1:808:A:THR:N  | 1:808:A:THR:CA | 1:808:A:THR:C | 14       | 1.61          |
| (1,172) | 1:848:A:LEU:N | 1:848:A:LEU:CA | 1:848:A:LEU:C  | 1:849:A:ARG:N | 6        | 1.4           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 14       | 1.29          |
| (1,125) | 1:817:A:SER:C | 1:818:A:ARG:N  | 1:818:A:ARG:CA | 1:818:A:ARG:C | 17       | 1.24          |
| (1,90)  | 1:797:A:SER:N | 1:797:A:SER:CA | 1:797:A:SER:C  | 1:798:A:ILE:N | 11       | 1.16          |
| (1,151) | 1:835:A:ILE:C | 1:836:A:LEU:N  | 1:836:A:LEU:CA | 1:836:A:LEU:C | 1        | 1.07          |