



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:54 AM UTC

PDB ID : 2MYU / pdb\_00002myu  
BMRB ID : 25243  
Title : An arsenate reductase in oxidized state  
Authors : Jin, C.; Hu, C.; Hu, Y.  
Deposited on : 2015-01-30

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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

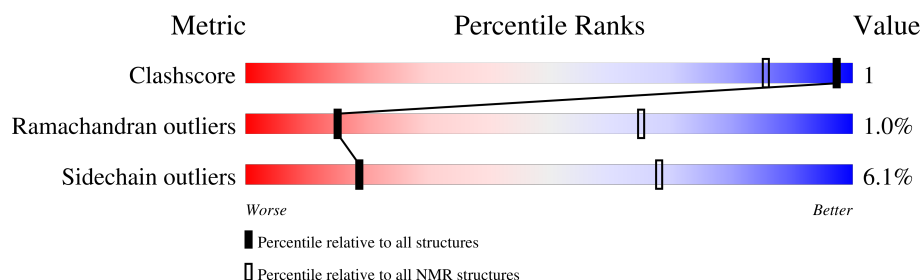
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 90%.

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     | 131    | <br>92% . . . |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:1-A:80, A:86-A:131 (126) | 0.45              | 2            |

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 2 clusters and 11 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1999 atoms, of which 992 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Glutaredoxin arsenate reductase.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 131      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1999  | 626 | 992 | 171 | 203 | 7 |       |

There are 3 discrepancies between the modelled and reference sequences:

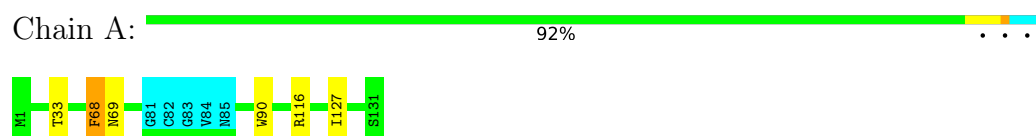
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 8       | SER      | CYS    | engineered mutation | UNP P74313 |
| A     | 13      | SER      | CYS    | engineered mutation | UNP P74313 |
| A     | 35      | SER      | CYS    | engineered mutation | UNP P74313 |

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

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

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

- Molecule 1: Glutaredoxin arsenate reductase

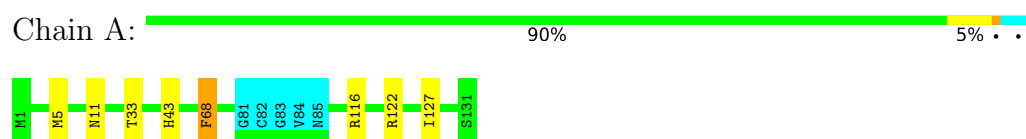


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

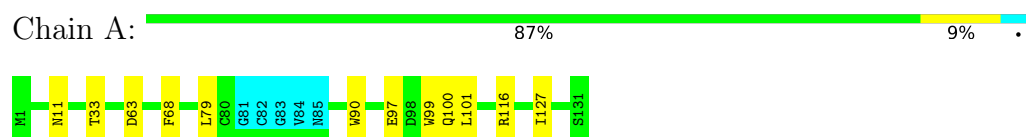
#### 4.2.1 Score per residue for model 1

- Molecule 1: Glutaredoxin arsenate reductase



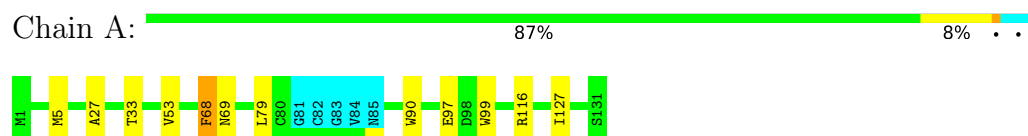
#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Glutaredoxin arsenate reductase



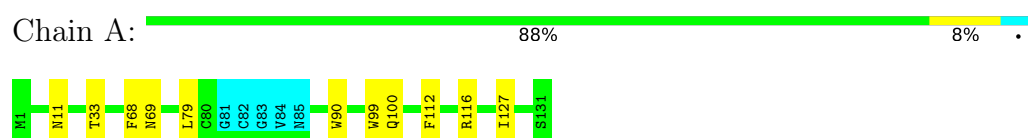
### 4.2.3 Score per residue for model 3

- Molecule 1: Glutaredoxin arsenate reductase



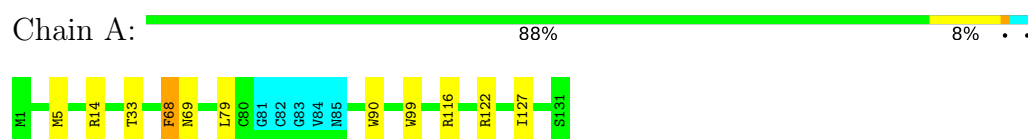
### 4.2.4 Score per residue for model 4

- Molecule 1: Glutaredoxin arsenate reductase



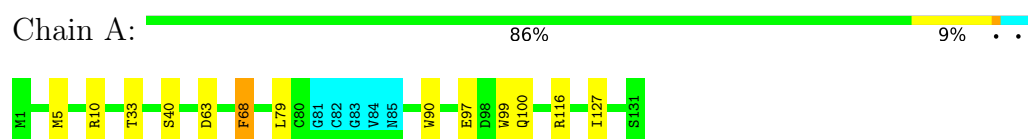
### 4.2.5 Score per residue for model 5

- Molecule 1: Glutaredoxin arsenate reductase



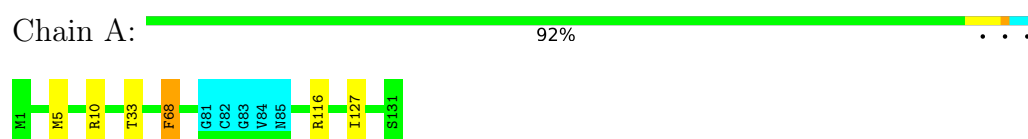
### 4.2.6 Score per residue for model 6

- Molecule 1: Glutaredoxin arsenate reductase



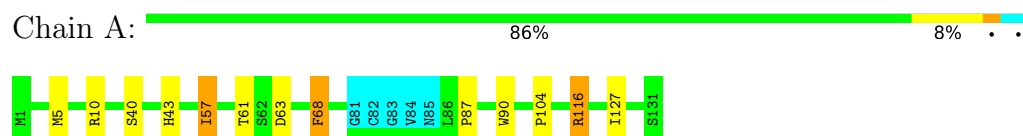
### 4.2.7 Score per residue for model 7

- Molecule 1: Glutaredoxin arsenate reductase



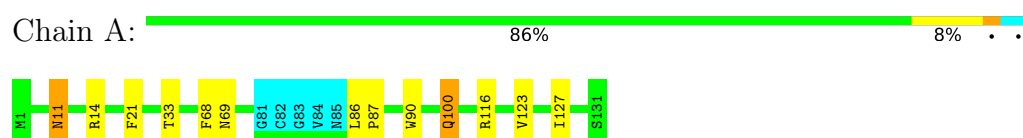
#### 4.2.8 Score per residue for model 8

- Molecule 1: Glutaredoxin arsenate reductase



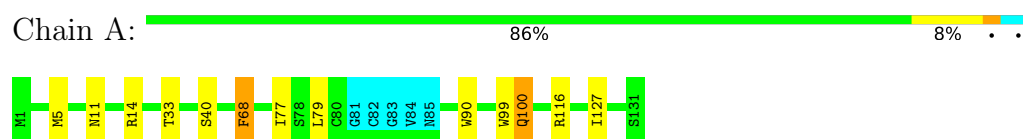
#### 4.2.9 Score per residue for model 9

- Molecule 1: Glutaredoxin arsenate reductase



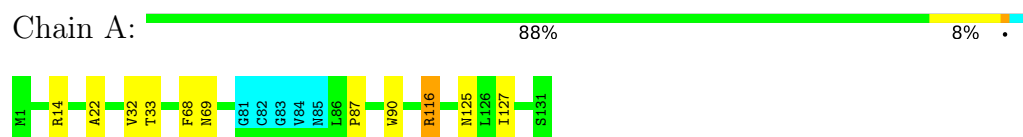
#### 4.2.10 Score per residue for model 10

- Molecule 1: Glutaredoxin arsenate reductase



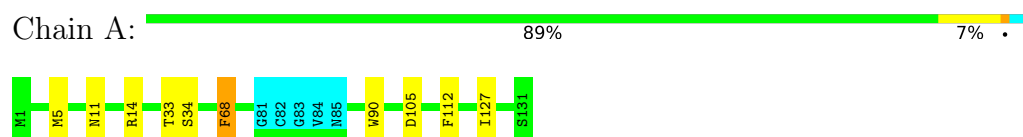
#### 4.2.11 Score per residue for model 11

- Molecule 1: Glutaredoxin arsenate reductase



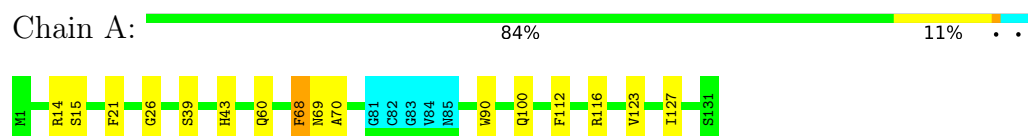
#### 4.2.12 Score per residue for model 12

- Molecule 1: Glutaredoxin arsenate reductase



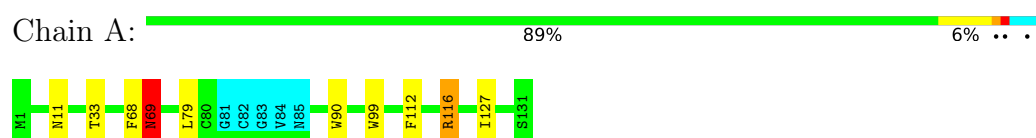
### 4.2.13 Score per residue for model 13

- Molecule 1: Glutaredoxin arsenate reductase



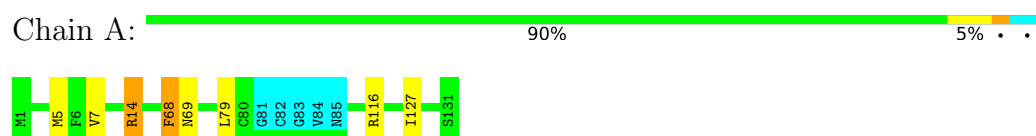
### 4.2.14 Score per residue for model 14

- Molecule 1: Glutaredoxin arsenate reductase



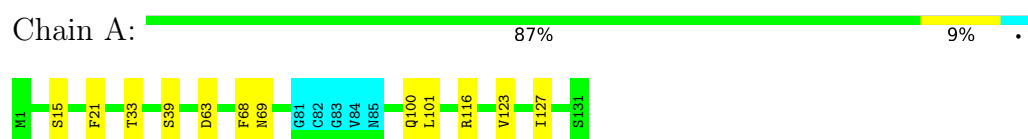
### 4.2.15 Score per residue for model 15

- Molecule 1: Glutaredoxin arsenate reductase



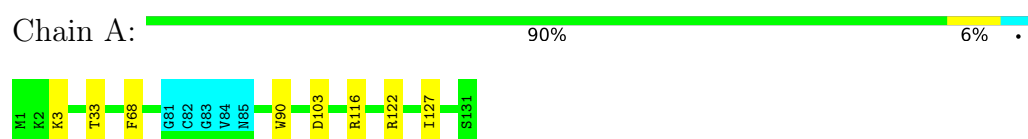
### 4.2.16 Score per residue for model 16

- Molecule 1: Glutaredoxin arsenate reductase



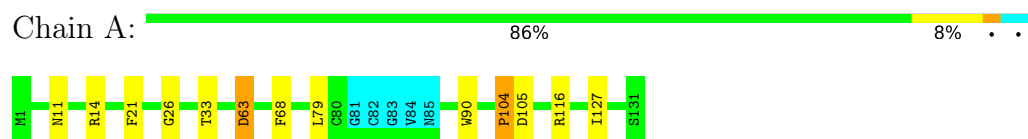
### 4.2.17 Score per residue for model 17

- Molecule 1: Glutaredoxin arsenate reductase



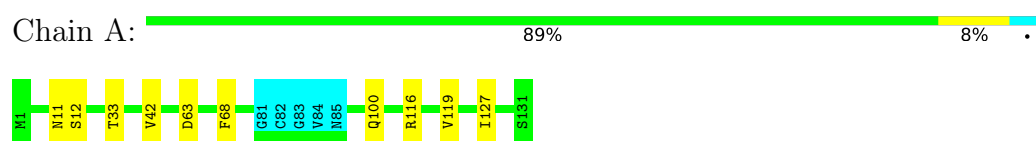
#### 4.2.18 Score per residue for model 18

- Molecule 1: Glutaredoxin arsenate reductase



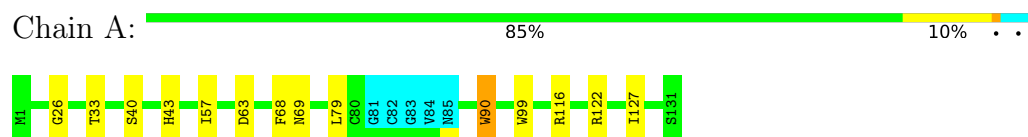
#### 4.2.19 Score per residue for model 19

- Molecule 1: Glutaredoxin arsenate reductase



#### 4.2.20 Score per residue for model 20

- Molecule 1: Glutaredoxin arsenate reductase



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| Amber         | refinement         |         |
| CYANA         | structure solution |         |

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                       | 1555           |
| Number of shifts mapped to atoms             | 1555           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 90%            |

## 6 Model quality

### 6.1 Standard geometry

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

| Mol | Chain | Bond lengths |                      | Bond angles |                       |
|-----|-------|--------------|----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                  |
| 1   | A     | 0.88±0.01    | 0±0/993 ( 0.0± 0.0%) | 1.37±0.03   | 2±1/1339 ( 0.2± 0.1%) |
| All | All   | 0.88         | 3/19860 ( 0.0%)      | 1.37        | 41/26780 ( 0.2%)      |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 0.4±0.6   |
| All | All   | 0         | 8         |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | A     | 87  | PRO  | CA-C  | 5.22 | 1.54        | 1.51     | 9      | 3     |

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     | 116 | ARG  | CD-NE-CZ  | 6.45 | 133.43      | 124.40   | 8      | 4     |
| 1   | A     | 90  | TRP  | CB-CG-CD2 | 6.01 | 135.22      | 126.80   | 12     | 2     |
| 1   | A     | 11  | ASN  | CA-C-N    | 5.47 | 127.55      | 120.44   | 9      | 7     |
| 1   | A     | 11  | ASN  | C-N-CA    | 5.47 | 127.55      | 120.44   | 9      | 7     |
| 1   | A     | 69  | ASN  | CA-CB-CG  | 5.39 | 117.99      | 112.60   | 14     | 1     |
| 1   | A     | 12  | SER  | N-CA-C    | 5.38 | 116.95      | 111.14   | 19     | 1     |
| 1   | A     | 119 | VAL  | CA-CB-CG2 | 5.35 | 119.50      | 110.40   | 19     | 1     |
| 1   | A     | 116 | ARG  | CA-CB-CG  | 5.33 | 124.77      | 114.10   | 10     | 1     |
| 1   | A     | 57  | ILE  | CA-C-N    | 5.28 | 127.89      | 120.28   | 8      | 1     |
| 1   | A     | 57  | ILE  | C-N-CA    | 5.28 | 127.89      | 120.28   | 8      | 1     |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 68  | PHE  | CA-CB-CG   | 5.28  | 119.08      | 113.80   | 13     | 1     |
| 1   | A     | 104 | PRO  | CA-C-N     | 5.28  | 131.62      | 121.54   | 18     | 1     |
| 1   | A     | 104 | PRO  | C-N-CA     | 5.28  | 131.62      | 121.54   | 18     | 1     |
| 1   | A     | 122 | ARG  | CD-NE-CZ   | 5.25  | 131.76      | 124.40   | 20     | 4     |
| 1   | A     | 60  | GLN  | OE1-CD-NE2 | -5.18 | 117.42      | 122.60   | 13     | 1     |
| 1   | A     | 43  | HIS  | CB-CG-CD2  | -5.16 | 124.49      | 131.20   | 20     | 4     |
| 1   | A     | 11  | ASN  | OD1-CG-ND2 | -5.11 | 117.49      | 122.60   | 4      | 1     |
| 1   | A     | 86  | LEU  | CA-C-N     | 5.02  | 123.33      | 119.66   | 9      | 1     |
| 1   | A     | 86  | LEU  | C-N-CA     | 5.02  | 123.33      | 119.66   | 9      | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 14  | ARG  | Sidechain | 5              |
| 1   | A     | 116 | ARG  | Sidechain | 2              |
| 1   | A     | 10  | ARG  | Sidechain | 1              |

## 6.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 978   | 967      | 967      | 1±1     |
| All | All   | 19560 | 19340    | 19340    | 24      |

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:5:MET:HE3  | 1:A:68:PHE:CD1  | 0.60     | 2.30        | 10     | 4     |
| 1:A:22:ALA:HB1 | 1:A:32:VAL:HG11 | 0.56     | 1.76        | 11     | 1     |
| 1:A:5:MET:HE3  | 1:A:68:PHE:CD2  | 0.48     | 2.43        | 7      | 5     |
| 1:A:11:ASN:ND2 | 1:A:63:ASP:H    | 0.44     | 2.10        | 19     | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:21:PHE:HB3  | 1:A:123:VAL:HG11 | 0.44     | 1.90        | 13     | 3     |
| 1:A:79:LEU:CD2  | 1:A:99:TRP:CE3   | 0.43     | 3.01        | 3      | 7     |
| 1:A:77:ILE:HG21 | 1:A:99:TRP:CE2   | 0.41     | 2.50        | 10     | 1     |
| 1:A:22:ALA:CB   | 1:A:32:VAL:HG11  | 0.41     | 2.45        | 11     | 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     | 124/131 (95%)   | 112±2 (90±2%) | 11±2 (9±2%) | 1±1 (1±1%) | 15          | 65 |
| All | All   | 2480/2620 (95%) | 2244 (90%)    | 211 (9%)    | 25 (1%)    | 15          | 65 |

All 12 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     | 100 | GLN  | 6              |
| 1   | A     | 40  | SER  | 4              |
| 1   | A     | 26  | GLY  | 3              |
| 1   | A     | 101 | LEU  | 2              |
| 1   | A     | 104 | PRO  | 2              |
| 1   | A     | 69  | ASN  | 2              |
| 1   | A     | 27  | ALA  | 1              |
| 1   | A     | 14  | ARG  | 1              |
| 1   | A     | 70  | ALA  | 1              |
| 1   | A     | 39  | SER  | 1              |
| 1   | A     | 105 | ASP  | 1              |
| 1   | A     | 42  | VAL  | 1              |

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

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

was analysed and the total number of residues.

| Mol | Chain | Analysed        | Rotameric     | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|-------------|----|
| 1   | A     | 110/113 (97%)   | 103±2 (94±1%) | 7±2 (6±1%) | 19          | 68 |
| All | All   | 2200/2260 (97%) | 2065 (94%)    | 135 (6%)   | 19          | 68 |

All 26 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     | 68  | PHE  | 20             |
| 1   | A     | 127 | ILE  | 20             |
| 1   | A     | 33  | THR  | 17             |
| 1   | A     | 116 | ARG  | 15             |
| 1   | A     | 90  | TRP  | 14             |
| 1   | A     | 69  | ASN  | 9              |
| 1   | A     | 63  | ASP  | 6              |
| 1   | A     | 100 | GLN  | 4              |
| 1   | A     | 112 | PHE  | 4              |
| 1   | A     | 97  | GLU  | 3              |
| 1   | A     | 79  | LEU  | 3              |
| 1   | A     | 14  | ARG  | 3              |
| 1   | A     | 10  | ARG  | 2              |
| 1   | A     | 57  | ILE  | 2              |
| 1   | A     | 15  | SER  | 2              |
| 1   | A     | 53  | VAL  | 1              |
| 1   | A     | 61  | THR  | 1              |
| 1   | A     | 11  | ASN  | 1              |
| 1   | A     | 125 | ASN  | 1              |
| 1   | A     | 34  | SER  | 1              |
| 1   | A     | 105 | ASP  | 1              |
| 1   | A     | 39  | SER  | 1              |
| 1   | A     | 7   | VAL  | 1              |
| 1   | A     | 3   | LYS  | 1              |
| 1   | A     | 103 | ASP  | 1              |
| 1   | A     | 21  | PHE  | 1              |

### 6.3.3 RNA ⓘ

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 90% for the well-defined parts and 90% 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                  | 1555 |
| Number of shifts mapped to atoms        | 1555 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 16   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 130      | $-0.88 \pm 0.21$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 119      | $0.33 \pm 0.17$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 122      | $-1.73 \pm 0.43$                | Should be applied          |
| $^{15}\text{N}$        | 123      | $0.73 \pm 0.38$                 | None needed (imprecise)    |

#### 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 90%, i.e. 1513 atoms were assigned a chemical shift out of a possible 1681. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 611/628 (97%) | 251/255 (98%) | 242/252 (96%)   | 118/121 (98%)   |
| Sidechain | 852/963 (88%) | 577/625 (92%) | 263/303 (87%)   | 12/35 (34%)     |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 50/90 (56%)     | 25/45 (56%)    | 23/42 (55%)     | 2/3 (67%)       |
| Overall  | 1513/1681 (90%) | 853/925 (92%)  | 528/597 (88%)   | 132/159 (83%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1555 atoms were assigned a chemical shift out of a possible 1728. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 637/655 (97%)   | 262/267 (98%)  | 252/262 (96%)   | 123/126 (98%)   |
| Sidechain | 868/983 (88%)   | 588/638 (92%)  | 267/309 (86%)   | 13/36 (36%)     |
| Aromatic  | 50/90 (56%)     | 25/45 (56%)    | 23/42 (55%)     | 2/3 (67%)       |
| Overall   | 1555/1728 (90%) | 875/950 (92%)  | 542/613 (88%)   | 138/165 (84%)   |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

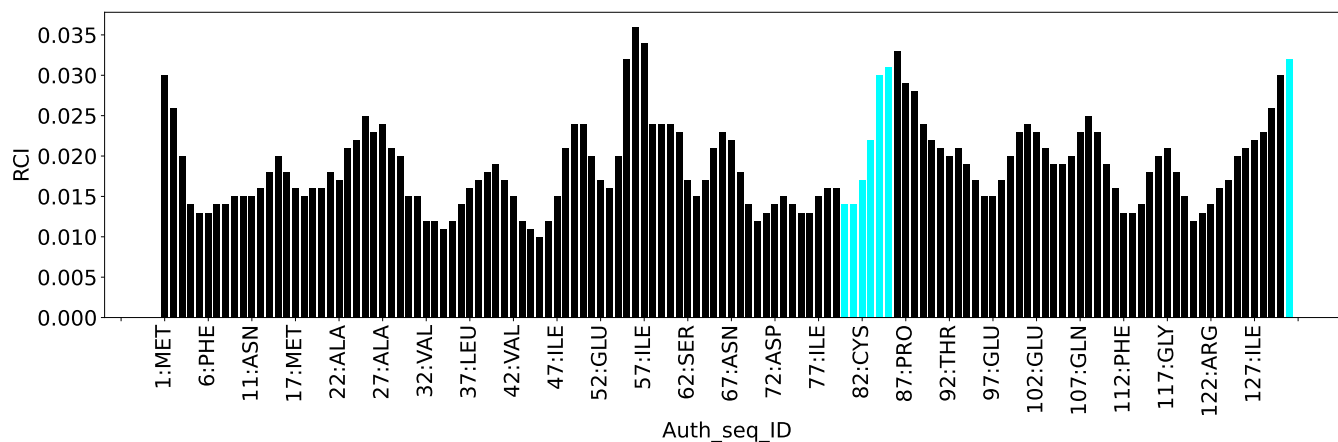
| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 68  | PHE  | CD2  | 115.55     | 125.53 – 137.61     | -13.3   |
| 1       | A     | 73  | TYR  | CD1  | 118.01     | 125.84 – 139.60     | -10.7   |
| 1       | A     | 73  | TYR  | CE1  | 130.20     | 111.24 – 124.66     | 9.1     |
| 1       | A     | 77  | ILE  | HG21 | -1.08      | -0.56 – 2.11        | -7.0    |
| 1       | A     | 77  | ILE  | HG22 | -1.08      | -0.56 – 2.11        | -7.0    |
| 1       | A     | 77  | ILE  | HG23 | -1.08      | -0.56 – 2.11        | -7.0    |
| 1       | A     | 70  | ALA  | HB1  | -0.29      | 0.14 – 2.58         | -6.8    |
| 1       | A     | 70  | ALA  | HB2  | -0.29      | 0.14 – 2.58         | -6.8    |
| 1       | A     | 70  | ALA  | HB3  | -0.29      | 0.14 – 2.58         | -6.8    |
| 1       | A     | 112 | PHE  | CZ   | 139.13     | 121.82 – 136.66     | 6.7     |
| 1       | A     | 68  | PHE  | CZ   | 120.24     | 121.82 – 136.66     | -6.1    |
| 1       | A     | 45  | THR  | H    | 11.80      | 5.19 – 11.27        | 5.9     |
| 1       | A     | 70  | ALA  | HA   | 1.86       | 2.13 – 6.34         | -5.7    |
| 1       | A     | 68  | PHE  | CE2  | 124.16     | 124.80 – 136.72     | -5.5    |
| 1       | A     | 122 | ARG  | HE   | 10.28      | 4.52 – 10.19        | 5.2     |
| 1       | A     | 104 | PRO  | HB3  | 0.22       | 0.25 – 3.76         | -5.1    |

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication

of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 3778  |
| Intra-residue ( $ i-j =0$ )                              | 1331  |
| Sequential ( $ i-j =1$ )                                 | 846   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 628   |
| Long range ( $ i-j \geq 5$ )                             | 972   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 1     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 28.8  |
| Number of long range restraints per residue <sup>1</sup> | 7.4   |

<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)  | 31.9                                   | 0.2     |
| 0.2-0.5 (Medium) | 29.5                                   | 0.5     |
| >0.5 (Large)     | 56.5                                   | 2.31    |

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

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

## 9 Distance violation analysis ⓘ

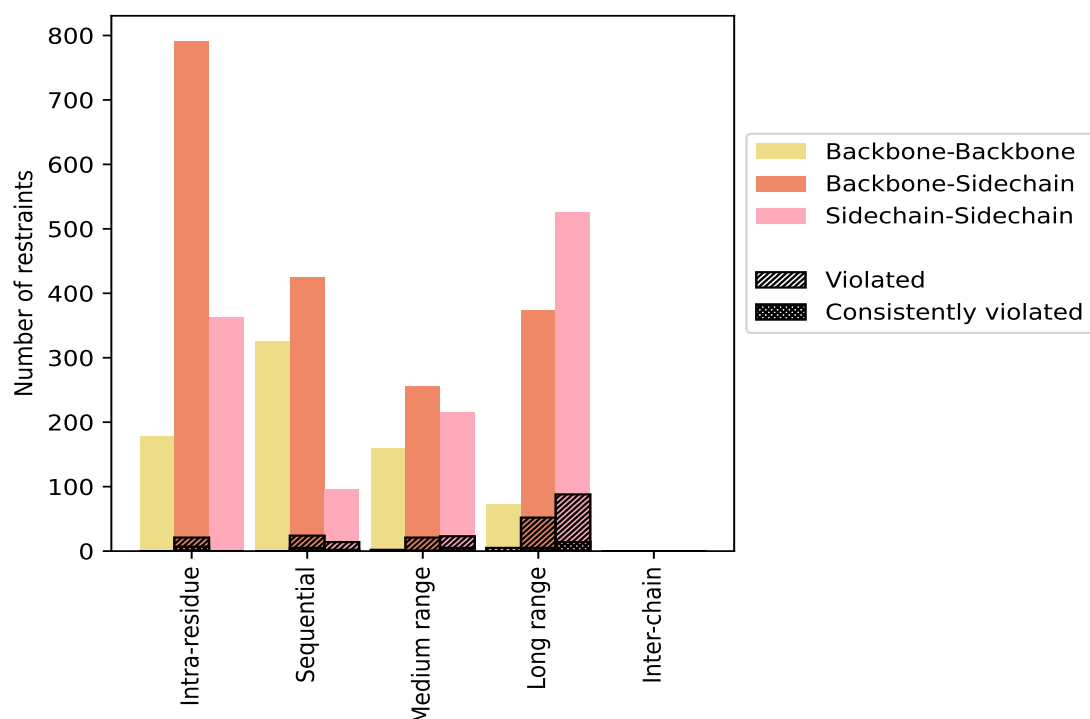
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>1331</b> | <b>35.2</b>    | <b>21</b>             | <b>1.6</b>     | <b>0.6</b>     | <b>7</b>                           | <b>0.5</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 178         | 4.7            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 791         | 20.9           | 21                    | 2.7            | 0.6            | 7                                  | 0.9            | 0.2            |
| Sidechain-Sidechain                                                         | 362         | 9.6            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>846</b>  | <b>22.4</b>    | <b>38</b>             | <b>4.5</b>     | <b>1.0</b>     | <b>7</b>                           | <b>0.8</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 326         | 8.6            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 425         | 11.2           | 24                    | 5.6            | 0.6            | 5                                  | 1.2            | 0.1            |
| Sidechain-Sidechain                                                         | 95          | 2.5            | 14                    | 14.7           | 0.4            | 2                                  | 2.1            | 0.1            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>628</b>  | <b>16.6</b>    | <b>46</b>             | <b>7.3</b>     | <b>1.2</b>     | <b>6</b>                           | <b>1.0</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 159         | 4.2            | 2                     | 1.3            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 255         | 6.7            | 21                    | 8.2            | 0.6            | 1                                  | 0.4            | 0.0            |
| Sidechain-Sidechain                                                         | 214         | 5.7            | 23                    | 10.7           | 0.6            | 5                                  | 2.3            | 0.1            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>972</b>  | <b>25.7</b>    | <b>145</b>            | <b>14.9</b>    | <b>3.8</b>     | <b>19</b>                          | <b>2.0</b>     | <b>0.5</b>     |
| Backbone-Backbone                                                           | 73          | 1.9            | 5                     | 6.8            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 373         | 9.9            | 52                    | 13.9           | 1.4            | 5                                  | 1.3            | 0.1            |
| Sidechain-Sidechain                                                         | 526         | 13.9           | 88                    | 16.7           | 2.3            | 14                                 | 2.7            | 0.4            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>1</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>3778</b> | <b>100.0</b>   | <b>250</b>            | <b>6.6</b>     | <b>6.6</b>     | <b>39</b>                          | <b>1.0</b>     | <b>1.0</b>     |
| Backbone-Backbone                                                           | 736         | 19.5           | 7                     | 1.0            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 1844        | 48.8           | 118                   | 6.4            | 3.1            | 18                                 | 1.0            | 0.5            |
| Sidechain-Sidechain                                                         | 1198        | 31.7           | 125                   | 10.4           | 3.3            | 21                                 | 1.8            | 0.6            |

<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        | 11                   | 22              | 24              | 73              | 0               | 130   | 0.63     | 2.28    | 0.55                | 0.4        |
| 2        | 10                   | 20              | 27              | 53              | 0               | 110   | 0.68     | 2.31    | 0.54                | 0.49       |
| 3        | 9                    | 20              | 25              | 61              | 0               | 115   | 0.67     | 2.27    | 0.56                | 0.43       |
| 4        | 10                   | 20              | 24              | 62              | 0               | 116   | 0.6      | 2.05    | 0.5                 | 0.4        |
| 5        | 10                   | 18              | 23              | 57              | 0               | 108   | 0.62     | 2.28    | 0.53                | 0.4        |
| 6        | 10                   | 22              | 25              | 71              | 0               | 128   | 0.57     | 2.01    | 0.5                 | 0.39       |
| 7        | 9                    | 18              | 22              | 61              | 0               | 110   | 0.65     | 2.05    | 0.54                | 0.43       |
| 8        | 11                   | 18              | 26              | 78              | 0               | 133   | 0.65     | 2.21    | 0.55                | 0.47       |
| 9        | 9                    | 21              | 25              | 65              | 0               | 120   | 0.62     | 2.2     | 0.52                | 0.4        |
| 10       | 8                    | 20              | 24              | 78              | 0               | 130   | 0.64     | 2.29    | 0.54                | 0.43       |

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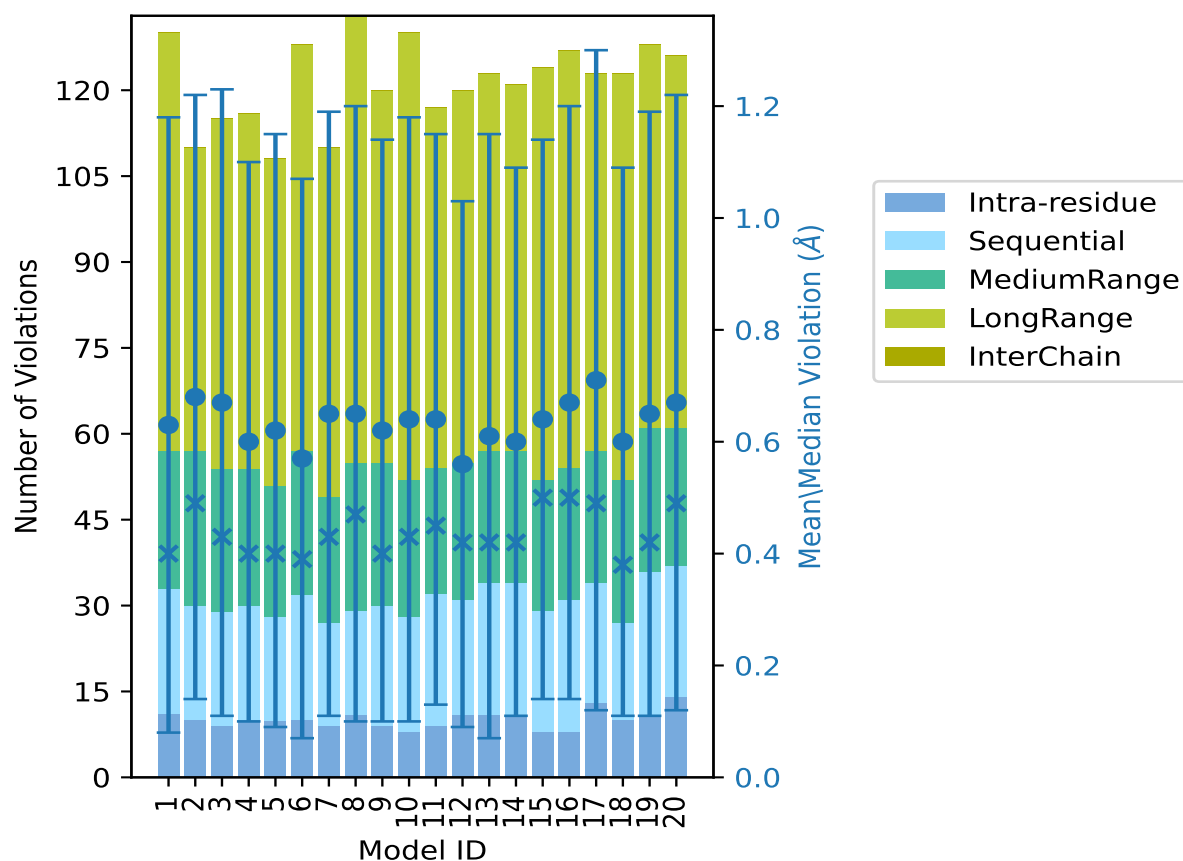
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 9                    | 23              | 22              | 63              | 0               | 117   | 0.64     | 2.15    | 0.51                | 0.45       |
| 12       | 11                   | 20              | 24              | 65              | 0               | 120   | 0.56     | 2.0     | 0.47                | 0.42       |
| 13       | 11                   | 23              | 23              | 66              | 0               | 123   | 0.61     | 2.18    | 0.54                | 0.42       |
| 14       | 11                   | 23              | 23              | 64              | 0               | 121   | 0.6      | 2.01    | 0.49                | 0.42       |
| 15       | 8                    | 21              | 23              | 72              | 0               | 124   | 0.64     | 2.18    | 0.5                 | 0.5        |
| 16       | 8                    | 23              | 23              | 73              | 0               | 127   | 0.67     | 2.12    | 0.53                | 0.5        |
| 17       | 13                   | 21              | 23              | 66              | 0               | 123   | 0.71     | 2.26    | 0.59                | 0.49       |
| 18       | 10                   | 17              | 25              | 71              | 0               | 123   | 0.6      | 2.24    | 0.49                | 0.38       |
| 19       | 11                   | 25              | 25              | 67              | 0               | 128   | 0.65     | 2.11    | 0.54                | 0.42       |
| 20       | 14                   | 23              | 24              | 65              | 0               | 126   | 0.67     | 2.14    | 0.55                | 0.49       |

<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

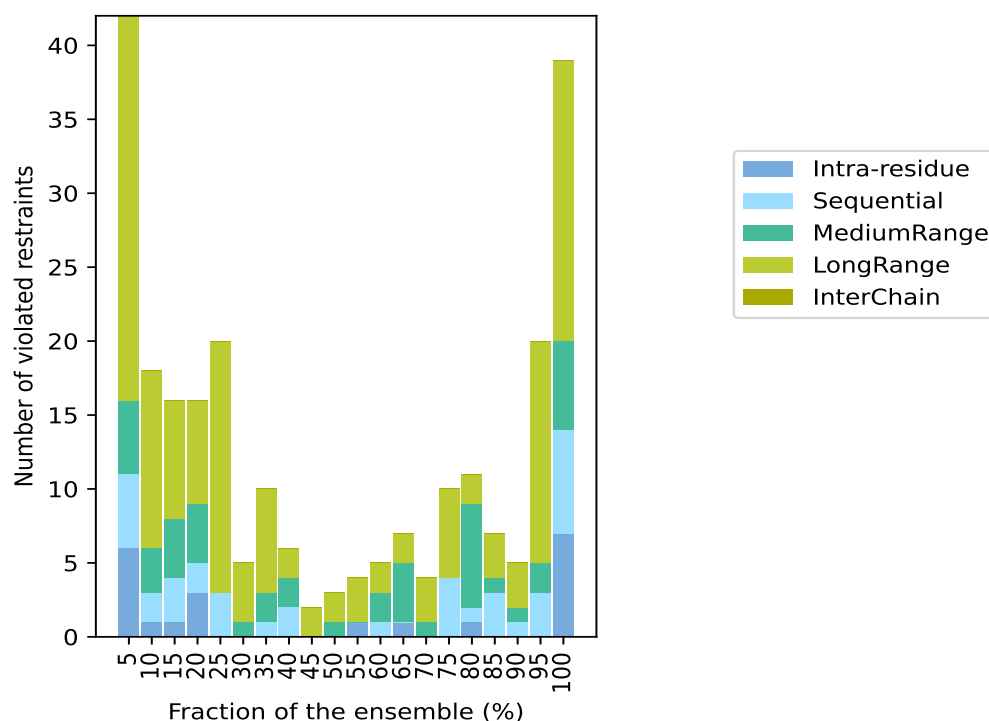
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3527(IR:1310, SQ:808, MR:582, LR:827, IC:0) restraints are 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>       | %     |
| 6                             | 5               | 5               | 26              | 0               | 42    | 1                        | 5.0   |
| 1                             | 2               | 3               | 12              | 0               | 18    | 2                        | 10.0  |
| 1                             | 3               | 4               | 8               | 0               | 16    | 3                        | 15.0  |
| 3                             | 2               | 4               | 7               | 0               | 16    | 4                        | 20.0  |
| 0                             | 3               | 0               | 17              | 0               | 20    | 5                        | 25.0  |
| 0                             | 0               | 1               | 4               | 0               | 5     | 6                        | 30.0  |
| 0                             | 1               | 2               | 7               | 0               | 10    | 7                        | 35.0  |
| 0                             | 2               | 2               | 2               | 0               | 6     | 8                        | 40.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 9                        | 45.0  |
| 0                             | 0               | 1               | 2               | 0               | 3     | 10                       | 50.0  |
| 1                             | 0               | 0               | 3               | 0               | 4     | 11                       | 55.0  |
| 0                             | 1               | 2               | 2               | 0               | 5     | 12                       | 60.0  |
| 1                             | 0               | 4               | 2               | 0               | 7     | 13                       | 65.0  |
| 0                             | 0               | 1               | 3               | 0               | 4     | 14                       | 70.0  |
| 0                             | 4               | 0               | 6               | 0               | 10    | 15                       | 75.0  |
| 1                             | 1               | 7               | 2               | 0               | 11    | 16                       | 80.0  |
| 0                             | 3               | 1               | 3               | 0               | 7     | 17                       | 85.0  |
| 0                             | 1               | 1               | 3               | 0               | 5     | 18                       | 90.0  |
| 0                             | 3               | 2               | 15              | 0               | 20    | 19                       | 95.0  |
| 7                             | 7               | 6               | 19              | 0               | 39    | 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

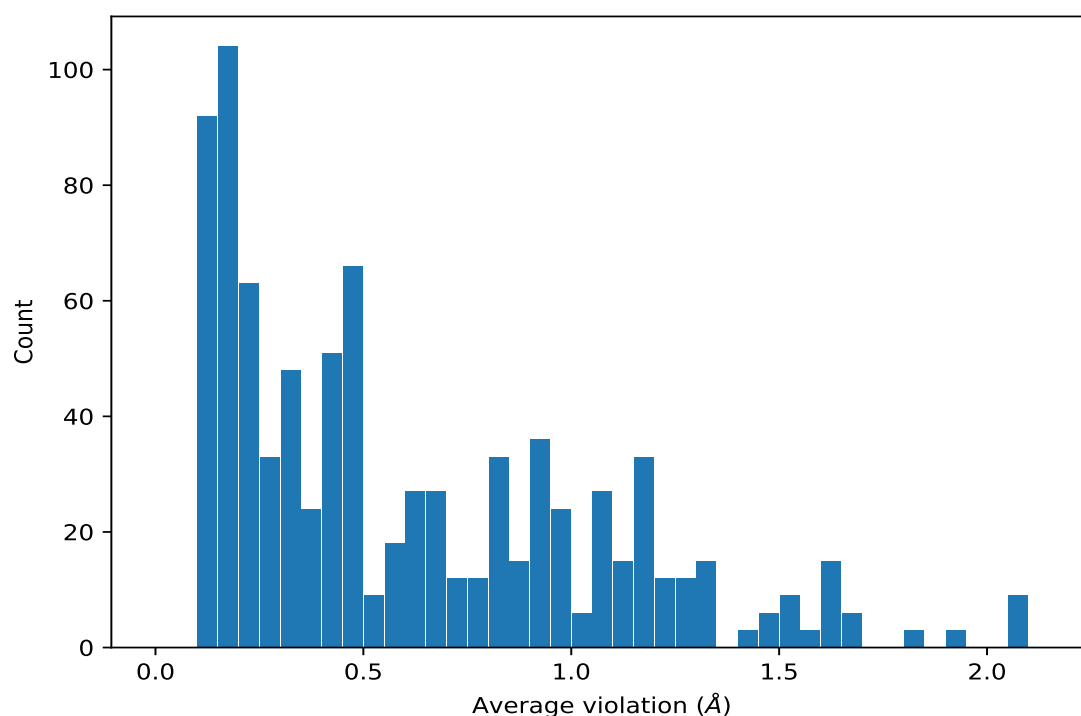
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 20                  | 2.07     | 0.17                | 2.08       |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 20                  | 2.07     | 0.17                | 2.08       |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 20                  | 2.07     | 0.17                | 2.08       |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 20                  | 2.07     | 0.17                | 2.08       |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 20                  | 2.07     | 0.17                | 2.08       |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 20                  | 2.07     | 0.17                | 2.08       |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 20                  | 1.65     | 0.11                | 1.66       |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 20                  | 1.65     | 0.11                | 1.66       |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 20                  | 1.65     | 0.11                | 1.66       |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 20                  | 1.64     | 0.51                | 1.73       |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 20                  | 1.64     | 0.51                | 1.73       |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 20                  | 1.64     | 0.51                | 1.73       |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 20                  | 1.64     | 0.51                | 1.73       |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 20                  | 1.64     | 0.51                | 1.73       |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 20                  | 1.64     | 0.51                | 1.73       |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 20                  | 1.56     | 0.58                | 1.94       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 20                  | 1.56     | 0.58                | 1.94       |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 20                  | 1.56     | 0.58                | 1.94       |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 20                  | 1.32     | 0.37                | 1.42       |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 20                  | 1.32     | 0.37                | 1.42       |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 20                  | 1.32     | 0.37                | 1.42       |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 20                  | 1.32     | 0.37                | 1.42       |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 20                  | 1.32     | 0.37                | 1.42       |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 20                  | 1.32     | 0.37                | 1.42       |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 20                  | 1.32     | 0.37                | 1.42       |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 20                  | 1.32     | 0.37                | 1.42       |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 20                  | 1.32     | 0.37                | 1.42       |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 20                  | 1.32     | 0.37                | 1.42       |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 20                  | 1.32     | 0.37                | 1.42       |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 20                  | 1.32     | 0.37                | 1.42       |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 20                  | 1.3      | 0.29                | 1.35       |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 20                  | 1.3      | 0.29                | 1.35       |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 20                  | 1.3      | 0.29                | 1.35       |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 20                  | 1.25     | 0.15                | 1.19       |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 20                  | 1.25     | 0.15                | 1.19       |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 20                  | 1.25     | 0.15                | 1.19       |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 20                  | 1.25     | 0.15                | 1.19       |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 20                  | 1.25     | 0.15                | 1.19       |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 20                  | 1.25     | 0.15                | 1.19       |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 20                  | 1.25     | 0.15                | 1.19       |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 20                  | 1.25     | 0.15                | 1.19       |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 20                  | 1.25     | 0.15                | 1.19       |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 20                  | 1.21     | 0.08                | 1.21       |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG21  | 20                  | 1.19     | 0.1                 | 1.16       |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG22  | 20                  | 1.19     | 0.1                 | 1.16       |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG23  | 20                  | 1.19     | 0.1                 | 1.16       |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG21  | 20                  | 1.19     | 0.1                 | 1.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG22  | 20                  | 1.19     | 0.1                 | 1.16       |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG23  | 20                  | 1.19     | 0.1                 | 1.16       |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG21  | 20                  | 1.19     | 0.1                 | 1.16       |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG22  | 20                  | 1.19     | 0.1                 | 1.16       |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG23  | 20                  | 1.19     | 0.1                 | 1.16       |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 20                  | 1.18     | 0.34                | 1.21       |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 20                  | 1.18     | 0.34                | 1.21       |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 20                  | 1.18     | 0.34                | 1.21       |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 20                  | 1.17     | 0.34                | 1.0        |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 20                  | 1.17     | 0.34                | 1.0        |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 20                  | 1.17     | 0.34                | 1.0        |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 20                  | 1.17     | 0.34                | 1.0        |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 20                  | 1.17     | 0.34                | 1.0        |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 20                  | 1.17     | 0.34                | 1.0        |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 20                  | 1.15     | 0.11                | 1.14       |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 20                  | 1.15     | 0.11                | 1.14       |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 20                  | 1.15     | 0.11                | 1.14       |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 20                  | 1.15     | 0.11                | 1.14       |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 20                  | 1.15     | 0.11                | 1.14       |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 20                  | 1.15     | 0.11                | 1.14       |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 20                  | 1.15     | 0.11                | 1.14       |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 20                  | 1.15     | 0.11                | 1.14       |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 20                  | 1.15     | 0.11                | 1.14       |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 20                  | 1.14     | 0.14                | 1.12       |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 20                  | 1.14     | 0.14                | 1.12       |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 20                  | 1.14     | 0.14                | 1.12       |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 20                  | 1.14     | 0.14                | 1.12       |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 20                  | 1.14     | 0.14                | 1.12       |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 20                  | 1.14     | 0.14                | 1.12       |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 20                  | 1.13     | 0.55                | 1.44       |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 20                  | 1.13     | 0.55                | 1.44       |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 20                  | 1.13     | 0.55                | 1.44       |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 20                  | 1.13     | 0.55                | 1.44       |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 20                  | 1.13     | 0.55                | 1.44       |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 20                  | 1.13     | 0.55                | 1.44       |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 20                  | 1.05     | 0.03                | 1.05       |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 20                  | 1.05     | 0.03                | 1.05       |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 20                  | 1.05     | 0.03                | 1.05       |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 20                  | 0.98     | 0.34                | 0.98       |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 20                  | 0.98     | 0.34                | 0.98       |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 20                  | 0.98     | 0.34                | 0.98       |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 20                  | 0.98     | 0.34                | 0.98       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 20                  | 0.98     | 0.34                | 0.98       |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 20                  | 0.98     | 0.34                | 0.98       |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 20                  | 0.98     | 0.34                | 0.98       |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 20                  | 0.98     | 0.34                | 0.98       |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 20                  | 0.98     | 0.34                | 0.98       |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 20                  | 0.98     | 0.34                | 0.98       |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 20                  | 0.98     | 0.34                | 0.98       |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 20                  | 0.98     | 0.34                | 0.98       |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 20                  | 0.93     | 0.21                | 0.93       |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 20                  | 0.93     | 0.21                | 0.93       |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 20                  | 0.93     | 0.21                | 0.93       |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 20                  | 0.93     | 0.21                | 0.93       |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 20                  | 0.93     | 0.21                | 0.93       |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 20                  | 0.93     | 0.21                | 0.93       |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 20                  | 0.93     | 0.21                | 0.88       |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 20                  | 0.93     | 0.21                | 0.88       |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 20                  | 0.93     | 0.21                | 0.88       |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 20                  | 0.92     | 0.34                | 1.0        |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 20                  | 0.92     | 0.34                | 1.0        |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 20                  | 0.92     | 0.34                | 1.0        |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 20                  | 0.92     | 0.34                | 1.0        |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 20                  | 0.92     | 0.34                | 1.0        |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 20                  | 0.92     | 0.34                | 1.0        |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 20                  | 0.88     | 0.14                | 0.86       |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 20                  | 0.88     | 0.14                | 0.86       |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 20                  | 0.88     | 0.14                | 0.86       |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 20                  | 0.88     | 0.14                | 0.86       |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22  | 20                  | 0.88     | 0.14                | 0.86       |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23  | 20                  | 0.88     | 0.14                | 0.86       |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21  | 20                  | 0.88     | 0.14                | 0.86       |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22  | 20                  | 0.88     | 0.14                | 0.86       |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23  | 20                  | 0.88     | 0.14                | 0.86       |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H    | 20                  | 0.74     | 0.11                | 0.72       |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H    | 20                  | 0.74     | 0.11                | 0.72       |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H    | 20                  | 0.74     | 0.11                | 0.72       |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11   | 20                  | 0.61     | 0.16                | 0.57       |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12   | 20                  | 0.61     | 0.16                | 0.57       |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13   | 20                  | 0.61     | 0.16                | 0.57       |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11   | 20                  | 0.61     | 0.16                | 0.57       |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12   | 20                  | 0.61     | 0.16                | 0.57       |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13   | 20                  | 0.61     | 0.16                | 0.57       |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 20                  | 0.56     | 0.05                | 0.56       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 20                  | 0.56     | 0.05                | 0.56       |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 20                  | 0.56     | 0.05                | 0.56       |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA    | 20                  | 0.4      | 0.01                | 0.4        |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA    | 20                  | 0.4      | 0.01                | 0.4        |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA    | 20                  | 0.4      | 0.01                | 0.4        |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 20                  | 0.4      | 0.01                | 0.4        |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12  | 20                  | 0.4      | 0.01                | 0.4        |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13  | 20                  | 0.4      | 0.01                | 0.4        |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 20                  | 0.38     | 0.02                | 0.37       |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 20                  | 0.38     | 0.02                | 0.37       |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 20                  | 0.38     | 0.02                | 0.37       |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2   | 20                  | 0.37     | 0.26                | 0.23       |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3   | 20                  | 0.37     | 0.26                | 0.23       |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2   | 20                  | 0.37     | 0.26                | 0.23       |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3   | 20                  | 0.37     | 0.26                | 0.23       |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2   | 20                  | 0.37     | 0.26                | 0.23       |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3   | 20                  | 0.37     | 0.26                | 0.23       |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 20                  | 0.33     | 0.01                | 0.33       |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 20                  | 0.33     | 0.01                | 0.33       |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 20                  | 0.33     | 0.01                | 0.33       |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 20                  | 0.25     | 0.02                | 0.25       |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 20                  | 0.21     | 0.02                | 0.2        |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 20                  | 0.21     | 0.02                | 0.2        |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 20                  | 0.21     | 0.02                | 0.2        |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 20                  | 0.21     | 0.02                | 0.2        |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 20                  | 0.21     | 0.02                | 0.2        |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 20                  | 0.21     | 0.02                | 0.2        |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 20                  | 0.18     | 0.02                | 0.17       |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 20                  | 0.18     | 0.02                | 0.17       |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21  | 20                  | 0.16     | 0.02                | 0.16       |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22  | 20                  | 0.16     | 0.02                | 0.16       |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23  | 20                  | 0.16     | 0.02                | 0.16       |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H    | 20                  | 0.15     | 0.01                | 0.16       |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H     | 20                  | 0.15     | 0.02                | 0.15       |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H     | 20                  | 0.15     | 0.02                | 0.15       |
| (1,634)  | 1:24:A:THR:H     | 1:24:A:THR:HB    | 20                  | 0.13     | 0.01                | 0.13       |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 19                  | 1.53     | 0.3                 | 1.56       |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 19                  | 1.53     | 0.3                 | 1.56       |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 19                  | 1.53     | 0.3                 | 1.56       |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 19                  | 1.53     | 0.3                 | 1.56       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22  | 19                  | 1.53     | 0.3                 | 1.56       |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23  | 19                  | 1.53     | 0.3                 | 1.56       |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21  | 19                  | 1.53     | 0.3                 | 1.56       |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22  | 19                  | 1.53     | 0.3                 | 1.56       |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23  | 19                  | 1.53     | 0.3                 | 1.56       |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11 | 19                  | 1.46     | 0.19                | 1.47       |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12 | 19                  | 1.46     | 0.19                | 1.47       |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13 | 19                  | 1.46     | 0.19                | 1.47       |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H    | 19                  | 1.46     | 0.19                | 1.47       |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H    | 19                  | 1.46     | 0.19                | 1.47       |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H    | 19                  | 1.46     | 0.19                | 1.47       |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21 | 19                  | 1.18     | 0.41                | 1.09       |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22 | 19                  | 1.18     | 0.41                | 1.09       |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23 | 19                  | 1.18     | 0.41                | 1.09       |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H    | 19                  | 1.16     | 0.16                | 1.13       |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H    | 19                  | 1.16     | 0.16                | 1.13       |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H    | 19                  | 1.16     | 0.16                | 1.13       |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2  | 19                  | 1.06     | 0.26                | 1.01       |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3  | 19                  | 1.06     | 0.26                | 1.01       |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2  | 19                  | 1.06     | 0.26                | 1.01       |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3  | 19                  | 1.06     | 0.26                | 1.01       |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2  | 19                  | 1.06     | 0.26                | 1.01       |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3  | 19                  | 1.06     | 0.26                | 1.01       |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG11 | 19                  | 1.05     | 0.14                | 1.08       |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG12 | 19                  | 1.05     | 0.14                | 1.08       |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG13 | 19                  | 1.05     | 0.14                | 1.08       |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG11 | 19                  | 1.05     | 0.14                | 1.08       |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG12 | 19                  | 1.05     | 0.14                | 1.08       |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG13 | 19                  | 1.05     | 0.14                | 1.08       |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 19                  | 0.83     | 0.33                | 0.78       |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 19                  | 0.72     | 0.16                | 0.67       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 19                  | 0.72     | 0.16                | 0.67       |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 19                  | 0.72     | 0.16                | 0.67       |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ    | 19                  | 0.6      | 0.2                 | 0.62       |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ    | 19                  | 0.6      | 0.2                 | 0.62       |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ    | 19                  | 0.6      | 0.2                 | 0.62       |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21 | 19                  | 0.5      | 0.12                | 0.51       |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG22 | 19                  | 0.5      | 0.12                | 0.51       |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG23 | 19                  | 0.5      | 0.12                | 0.51       |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1   | 19                  | 0.49     | 0.16                | 0.42       |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2   | 19                  | 0.49     | 0.16                | 0.42       |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1   | 19                  | 0.49     | 0.16                | 0.42       |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2   | 19                  | 0.49     | 0.16                | 0.42       |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1   | 19                  | 0.49     | 0.16                | 0.42       |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2   | 19                  | 0.49     | 0.16                | 0.42       |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11 | 19                  | 0.49     | 0.16                | 0.42       |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12 | 19                  | 0.49     | 0.16                | 0.42       |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13 | 19                  | 0.49     | 0.16                | 0.42       |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11 | 19                  | 0.49     | 0.16                | 0.42       |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12 | 19                  | 0.49     | 0.16                | 0.42       |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13 | 19                  | 0.49     | 0.16                | 0.42       |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11  | 19                  | 0.48     | 0.51                | 0.26       |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12  | 19                  | 0.48     | 0.51                | 0.26       |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13  | 19                  | 0.48     | 0.51                | 0.26       |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11  | 19                  | 0.48     | 0.51                | 0.26       |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12  | 19                  | 0.48     | 0.51                | 0.26       |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13  | 19                  | 0.48     | 0.51                | 0.26       |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11  | 19                  | 0.48     | 0.51                | 0.26       |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12  | 19                  | 0.48     | 0.51                | 0.26       |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13  | 19                  | 0.48     | 0.51                | 0.26       |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11 | 19                  | 0.31     | 0.11                | 0.29       |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG12 | 19                  | 0.31     | 0.11                | 0.29       |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG13 | 19                  | 0.31     | 0.11                | 0.29       |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG21 | 19                  | 0.3      | 0.13                | 0.29       |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG22 | 19                  | 0.3      | 0.13                | 0.29       |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG23 | 19                  | 0.3      | 0.13                | 0.29       |
| (1,793)  | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB   | 19                  | 0.17     | 0.01                | 0.17       |
| (1,793)  | 1:31:A:ALA:HB2   | 1:32:A:VAL:HB   | 19                  | 0.17     | 0.01                | 0.17       |
| (1,793)  | 1:31:A:ALA:HB3   | 1:32:A:VAL:HB   | 19                  | 0.17     | 0.01                | 0.17       |
| (1,991)  | 1:57:A:ILE:H     | 1:42:A:VAL:HB   | 19                  | 0.15     | 0.04                | 0.15       |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA2  | 19                  | 0.13     | 0.02                | 0.13       |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA3  | 19                  | 0.13     | 0.02                | 0.13       |
| (1,877)  | 1:5:A:MET:HG3    | 1:36:A:GLY:HA2  | 19                  | 0.13     | 0.02                | 0.13       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA3   | 19                  | 0.13     | 0.02                | 0.13       |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG11  | 18                  | 0.9      | 0.41                | 0.91       |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG12  | 18                  | 0.9      | 0.41                | 0.91       |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG13  | 18                  | 0.9      | 0.41                | 0.91       |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG21  | 18                  | 0.59     | 0.15                | 0.56       |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG22  | 18                  | 0.59     | 0.15                | 0.56       |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG23  | 18                  | 0.59     | 0.15                | 0.56       |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG21  | 18                  | 0.59     | 0.15                | 0.56       |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG22  | 18                  | 0.59     | 0.15                | 0.56       |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG23  | 18                  | 0.59     | 0.15                | 0.56       |
| (1,812)  | 1:4:A:VAL:HG23  | 1:32:A:VAL:HG21  | 18                  | 0.59     | 0.15                | 0.56       |
| (1,812)  | 1:4:A:VAL:HG23  | 1:32:A:VAL:HG22  | 18                  | 0.59     | 0.15                | 0.56       |
| (1,812)  | 1:4:A:VAL:HG23  | 1:32:A:VAL:HG23  | 18                  | 0.59     | 0.15                | 0.56       |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD11  | 18                  | 0.49     | 0.21                | 0.44       |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD12  | 18                  | 0.49     | 0.21                | 0.44       |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD13  | 18                  | 0.49     | 0.21                | 0.44       |
| (1,1776) | 1:37:A:LEU:HD11 | 1:86:A:LEU:HA    | 18                  | 0.49     | 0.21                | 0.44       |
| (1,1776) | 1:37:A:LEU:HD12 | 1:86:A:LEU:HA    | 18                  | 0.49     | 0.21                | 0.44       |
| (1,1776) | 1:37:A:LEU:HD13 | 1:86:A:LEU:HA    | 18                  | 0.49     | 0.21                | 0.44       |
| (1,649)  | 1:24:A:THR:HG21 | 1:25:A:LEU:HA    | 18                  | 0.12     | 0.01                | 0.12       |
| (1,649)  | 1:24:A:THR:HG22 | 1:25:A:LEU:HA    | 18                  | 0.12     | 0.01                | 0.12       |
| (1,649)  | 1:24:A:THR:HG23 | 1:25:A:LEU:HA    | 18                  | 0.12     | 0.01                | 0.12       |
| (1,256)  | 1:3:A:LYS:HA    | 1:4:A:VAL:HG11   | 17                  | 1.84     | 0.42                | 1.95       |
| (1,256)  | 1:3:A:LYS:HA    | 1:4:A:VAL:HG12   | 17                  | 1.84     | 0.42                | 1.95       |
| (1,256)  | 1:3:A:LYS:HA    | 1:4:A:VAL:HG13   | 17                  | 1.84     | 0.42                | 1.95       |
| (1,243)  | 1:75:A:VAL:HG21 | 1:4:A:VAL:HB     | 17                  | 0.93     | 0.16                | 0.95       |
| (1,243)  | 1:75:A:VAL:HG22 | 1:4:A:VAL:HB     | 17                  | 0.93     | 0.16                | 0.95       |
| (1,243)  | 1:75:A:VAL:HG23 | 1:4:A:VAL:HB     | 17                  | 0.93     | 0.16                | 0.95       |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG21   | 17                  | 0.83     | 0.14                | 0.87       |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG22   | 17                  | 0.83     | 0.14                | 0.87       |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG23   | 17                  | 0.83     | 0.14                | 0.87       |
| (1,3349) | 1:4:A:VAL:HG21  | 1:77:A:ILE:H     | 17                  | 0.83     | 0.14                | 0.87       |
| (1,3349) | 1:4:A:VAL:HG22  | 1:77:A:ILE:H     | 17                  | 0.83     | 0.14                | 0.87       |
| (1,3349) | 1:4:A:VAL:HG23  | 1:77:A:ILE:H     | 17                  | 0.83     | 0.14                | 0.87       |
| (1,274)  | 1:5:A:MET:H     | 1:4:A:VAL:HG21   | 17                  | 0.5      | 0.04                | 0.51       |
| (1,274)  | 1:5:A:MET:H     | 1:4:A:VAL:HG22   | 17                  | 0.5      | 0.04                | 0.51       |
| (1,274)  | 1:5:A:MET:H     | 1:4:A:VAL:HG23   | 17                  | 0.5      | 0.04                | 0.51       |
| (1,2431) | 1:122:A:ARG:HD2 | 1:119:A:VAL:HG21 | 17                  | 0.46     | 0.48                | 0.25       |
| (1,2431) | 1:122:A:ARG:HD2 | 1:119:A:VAL:HG22 | 17                  | 0.46     | 0.48                | 0.25       |
| (1,2431) | 1:122:A:ARG:HD2 | 1:119:A:VAL:HG23 | 17                  | 0.46     | 0.48                | 0.25       |
| (1,2431) | 1:122:A:ARG:HD3 | 1:119:A:VAL:HG21 | 17                  | 0.46     | 0.48                | 0.25       |
| (1,2431) | 1:122:A:ARG:HD3 | 1:119:A:VAL:HG22 | 17                  | 0.46     | 0.48                | 0.25       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 17                  | 0.46     | 0.48                | 0.25       |
| (1,633)  | 1:62:A:SER:HA    | 1:61:A:THR:HB    | 17                  | 0.15     | 0.03                | 0.15       |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 16                  | 1.04     | 0.08                | 1.02       |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 16                  | 1.04     | 0.08                | 1.02       |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 16                  | 1.04     | 0.08                | 1.02       |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 16                  | 1.04     | 0.08                | 1.02       |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 16                  | 1.04     | 0.08                | 1.02       |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 16                  | 1.04     | 0.08                | 1.02       |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21   | 16                  | 0.76     | 0.08                | 0.74       |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22   | 16                  | 0.76     | 0.08                | 0.74       |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23   | 16                  | 0.76     | 0.08                | 0.74       |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21   | 16                  | 0.76     | 0.08                | 0.74       |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22   | 16                  | 0.76     | 0.08                | 0.74       |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23   | 16                  | 0.76     | 0.08                | 0.74       |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11  | 16                  | 0.6      | 0.37                | 0.49       |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12  | 16                  | 0.6      | 0.37                | 0.49       |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13  | 16                  | 0.6      | 0.37                | 0.49       |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11  | 16                  | 0.6      | 0.37                | 0.49       |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12  | 16                  | 0.6      | 0.37                | 0.49       |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13  | 16                  | 0.6      | 0.37                | 0.49       |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA    | 16                  | 0.43     | 0.36                | 0.3        |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA    | 16                  | 0.43     | 0.36                | 0.3        |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA    | 16                  | 0.43     | 0.36                | 0.3        |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG11   | 16                  | 0.41     | 0.02                | 0.41       |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG12   | 16                  | 0.41     | 0.02                | 0.41       |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG13   | 16                  | 0.41     | 0.02                | 0.41       |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG11 | 16                  | 0.39     | 0.11                | 0.38       |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG12 | 16                  | 0.39     | 0.11                | 0.38       |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG13 | 16                  | 0.39     | 0.11                | 0.38       |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 16                  | 0.36     | 0.1                 | 0.36       |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 16                  | 0.36     | 0.1                 | 0.36       |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 16                  | 0.36     | 0.1                 | 0.36       |
| (1,405)  | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB   | 16                  | 0.29     | 0.09                | 0.3        |
| (1,405)  | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB   | 16                  | 0.29     | 0.09                | 0.3        |
| (1,405)  | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB   | 16                  | 0.29     | 0.09                | 0.3        |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 16                  | 0.25     | 0.05                | 0.26       |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 16                  | 0.25     | 0.05                | 0.26       |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 16                  | 0.25     | 0.05                | 0.26       |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 16                  | 0.25     | 0.05                | 0.26       |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 16                  | 0.25     | 0.05                | 0.26       |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 16                  | 0.25     | 0.05                | 0.26       |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 16                  | 0.25     | 0.05                | 0.26       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 16                  | 0.25     | 0.05                | 0.26       |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 16                  | 0.25     | 0.05                | 0.26       |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 16                  | 0.24     | 0.06                | 0.24       |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 16                  | 0.24     | 0.06                | 0.24       |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 16                  | 0.24     | 0.06                | 0.24       |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H     | 16                  | 0.13     | 0.02                | 0.13       |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H     | 16                  | 0.13     | 0.02                | 0.13       |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11  | 15                  | 0.95     | 0.19                | 0.9        |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12  | 15                  | 0.95     | 0.19                | 0.9        |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13  | 15                  | 0.95     | 0.19                | 0.9        |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11  | 15                  | 0.95     | 0.19                | 0.9        |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12  | 15                  | 0.95     | 0.19                | 0.9        |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13  | 15                  | 0.95     | 0.19                | 0.9        |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1   | 15                  | 0.75     | 0.93                | 0.12       |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1   | 15                  | 0.75     | 0.93                | 0.12       |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1   | 15                  | 0.75     | 0.93                | 0.12       |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H     | 15                  | 0.68     | 0.17                | 0.69       |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H     | 15                  | 0.68     | 0.17                | 0.69       |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H     | 15                  | 0.68     | 0.17                | 0.69       |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA    | 15                  | 0.62     | 0.06                | 0.61       |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA    | 15                  | 0.62     | 0.06                | 0.61       |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA    | 15                  | 0.62     | 0.06                | 0.61       |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 15                  | 0.29     | 0.12                | 0.35       |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 15                  | 0.29     | 0.12                | 0.35       |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 15                  | 0.29     | 0.12                | 0.35       |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H     | 15                  | 0.29     | 0.15                | 0.25       |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H     | 15                  | 0.29     | 0.15                | 0.25       |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H     | 15                  | 0.29     | 0.15                | 0.25       |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H    | 15                  | 0.18     | 0.05                | 0.16       |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H    | 15                  | 0.18     | 0.05                | 0.16       |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H    | 15                  | 0.18     | 0.05                | 0.16       |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1    | 15                  | 0.15     | 0.02                | 0.16       |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2    | 15                  | 0.15     | 0.02                | 0.16       |
| (1,433)  | 1:50:A:MET:HE1   | 1:16:A:GLN:HA    | 15                  | 0.13     | 0.02                | 0.12       |
| (1,433)  | 1:50:A:MET:HE2   | 1:16:A:GLN:HA    | 15                  | 0.13     | 0.02                | 0.12       |
| (1,433)  | 1:50:A:MET:HE3   | 1:16:A:GLN:HA    | 15                  | 0.13     | 0.02                | 0.12       |
| (1,1355) | 1:47:A:ILE:HG21  | 1:58:A:SER:HA    | 15                  | 0.12     | 0.01                | 0.12       |
| (1,1355) | 1:47:A:ILE:HG22  | 1:58:A:SER:HA    | 15                  | 0.12     | 0.01                | 0.12       |
| (1,1355) | 1:47:A:ILE:HG23  | 1:58:A:SER:HA    | 15                  | 0.12     | 0.01                | 0.12       |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA    | 14                  | 0.43     | 0.15                | 0.43       |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA    | 14                  | 0.43     | 0.15                | 0.43       |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA    | 14                  | 0.43     | 0.15                | 0.43       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 14                  | 0.43     | 0.15                | 0.43       |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 14                  | 0.43     | 0.15                | 0.43       |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 14                  | 0.43     | 0.15                | 0.43       |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2   | 14                  | 0.18     | 0.03                | 0.18       |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3   | 14                  | 0.18     | 0.03                | 0.18       |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2   | 14                  | 0.18     | 0.03                | 0.18       |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3   | 14                  | 0.18     | 0.03                | 0.18       |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE1   | 14                  | 0.12     | 0.01                | 0.12       |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE2   | 14                  | 0.12     | 0.01                | 0.12       |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 13                  | 1.42     | 0.06                | 1.4        |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 13                  | 1.42     | 0.06                | 1.4        |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 13                  | 1.42     | 0.06                | 1.4        |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 13                  | 0.42     | 0.06                | 0.4        |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG12 | 13                  | 0.42     | 0.06                | 0.4        |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG13 | 13                  | 0.42     | 0.06                | 0.4        |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 13                  | 0.27     | 0.02                | 0.28       |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 13                  | 0.27     | 0.02                | 0.28       |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 13                  | 0.27     | 0.02                | 0.28       |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG21   | 13                  | 0.22     | 0.09                | 0.21       |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG22   | 13                  | 0.22     | 0.09                | 0.21       |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG23   | 13                  | 0.22     | 0.09                | 0.21       |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA   | 13                  | 0.21     | 0.09                | 0.16       |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA   | 13                  | 0.21     | 0.09                | 0.16       |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA   | 13                  | 0.21     | 0.09                | 0.16       |
| (1,448)  | 1:19:A:GLU:H     | 1:16:A:GLN:HB2   | 13                  | 0.16     | 0.04                | 0.15       |
| (1,448)  | 1:19:A:GLU:H     | 1:16:A:GLN:HB3   | 13                  | 0.16     | 0.04                | 0.15       |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H    | 13                  | 0.13     | 0.04                | 0.12       |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H    | 13                  | 0.13     | 0.04                | 0.12       |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11  | 12                  | 0.58     | 0.57                | 0.2        |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12  | 12                  | 0.58     | 0.57                | 0.2        |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13  | 12                  | 0.58     | 0.57                | 0.2        |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H     | 12                  | 0.14     | 0.03                | 0.14       |
| (1,928)  | 1:40:A:SER:HA    | 1:38:A:GLU:HA    | 12                  | 0.14     | 0.04                | 0.12       |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2   | 12                  | 0.13     | 0.05                | 0.12       |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3   | 12                  | 0.13     | 0.05                | 0.12       |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H     | 12                  | 0.12     | 0.02                | 0.11       |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H     | 12                  | 0.12     | 0.02                | 0.11       |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG11   | 11                  | 0.55     | 0.48                | 0.31       |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG12   | 11                  | 0.55     | 0.48                | 0.31       |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG13   | 11                  | 0.55     | 0.48                | 0.31       |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H     | 11                  | 0.15     | 0.03                | 0.16       |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H     | 11                  | 0.15     | 0.03                | 0.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2   | 11                  | 0.14     | 0.03                | 0.15       |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3   | 11                  | 0.14     | 0.03                | 0.15       |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2   | 11                  | 0.14     | 0.03                | 0.15       |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3   | 11                  | 0.14     | 0.03                | 0.15       |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1   | 11                  | 0.12     | 0.02                | 0.12       |
| (1,1756) | 1:86:A:LEU:HD11  | 1:84:A:VAL:HA    | 10                  | 0.31     | 0.12                | 0.28       |
| (1,1756) | 1:86:A:LEU:HD12  | 1:84:A:VAL:HA    | 10                  | 0.31     | 0.12                | 0.28       |
| (1,1756) | 1:86:A:LEU:HD13  | 1:84:A:VAL:HA    | 10                  | 0.31     | 0.12                | 0.28       |
| (1,823)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG21  | 10                  | 0.21     | 0.29                | 0.11       |
| (1,823)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG22  | 10                  | 0.21     | 0.29                | 0.11       |
| (1,823)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG23  | 10                  | 0.21     | 0.29                | 0.11       |
| (1,823)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG21  | 10                  | 0.21     | 0.29                | 0.11       |
| (1,823)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG22  | 10                  | 0.21     | 0.29                | 0.11       |
| (1,823)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG23  | 10                  | 0.21     | 0.29                | 0.11       |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG2   | 10                  | 0.21     | 0.11                | 0.17       |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG3   | 10                  | 0.21     | 0.11                | 0.17       |
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG2   | 10                  | 0.21     | 0.11                | 0.17       |
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG3   | 10                  | 0.21     | 0.11                | 0.17       |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG2   | 10                  | 0.21     | 0.11                | 0.17       |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG3   | 10                  | 0.21     | 0.11                | 0.17       |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD21  | 9                   | 0.44     | 0.13                | 0.38       |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD22  | 9                   | 0.44     | 0.13                | 0.38       |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD23  | 9                   | 0.44     | 0.13                | 0.38       |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD21  | 9                   | 0.44     | 0.13                | 0.38       |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD22  | 9                   | 0.44     | 0.13                | 0.38       |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD23  | 9                   | 0.44     | 0.13                | 0.38       |
| (1,744)  | 1:1:A:MET:HB2    | 1:30:A:ILE:HB    | 9                   | 0.13     | 0.01                | 0.12       |
| (1,744)  | 1:1:A:MET:HB3    | 1:30:A:ILE:HB    | 9                   | 0.13     | 0.01                | 0.12       |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 8                   | 0.46     | 0.09                | 0.48       |
| (1,2649) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HA   | 8                   | 0.16     | 0.05                | 0.16       |
| (1,2649) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HA   | 8                   | 0.16     | 0.05                | 0.16       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2649) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HA  | 8                   | 0.16     | 0.05                | 0.16       |
| (1,2653) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HB  | 8                   | 0.16     | 0.06                | 0.15       |
| (1,2653) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HB  | 8                   | 0.16     | 0.06                | 0.15       |
| (1,2653) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HB  | 8                   | 0.16     | 0.06                | 0.15       |
| (1,826)  | 1:5:A:MET:HA     | 1:33:A:THR:HA   | 8                   | 0.15     | 0.04                | 0.13       |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB2  | 8                   | 0.11     | 0.01                | 0.11       |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB3  | 8                   | 0.11     | 0.01                | 0.11       |
| (1,845)  | 1:79:A:LEU:HD11  | 1:34:A:SER:HA   | 7                   | 0.84     | 0.52                | 0.86       |
| (1,845)  | 1:79:A:LEU:HD12  | 1:34:A:SER:HA   | 7                   | 0.84     | 0.52                | 0.86       |
| (1,845)  | 1:79:A:LEU:HD13  | 1:34:A:SER:HA   | 7                   | 0.84     | 0.52                | 0.86       |
| (1,144)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HZ    | 7                   | 0.81     | 0.18                | 0.81       |
| (1,144)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HZ    | 7                   | 0.81     | 0.18                | 0.81       |
| (1,144)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HZ    | 7                   | 0.81     | 0.18                | 0.81       |
| (1,142)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE1   | 7                   | 0.67     | 0.13                | 0.69       |
| (1,142)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE2   | 7                   | 0.67     | 0.13                | 0.69       |
| (1,142)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE1   | 7                   | 0.67     | 0.13                | 0.69       |
| (1,142)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE2   | 7                   | 0.67     | 0.13                | 0.69       |
| (1,142)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE1   | 7                   | 0.67     | 0.13                | 0.69       |
| (1,142)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE2   | 7                   | 0.67     | 0.13                | 0.69       |
| (1,2746) | 1:119:A:VAL:HG21 | 1:15:A:SER:HA   | 7                   | 0.53     | 0.37                | 0.28       |
| (1,2746) | 1:119:A:VAL:HG22 | 1:15:A:SER:HA   | 7                   | 0.53     | 0.37                | 0.28       |
| (1,2746) | 1:119:A:VAL:HG23 | 1:15:A:SER:HA   | 7                   | 0.53     | 0.37                | 0.28       |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD11 | 7                   | 0.33     | 0.3                 | 0.2        |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD12 | 7                   | 0.33     | 0.3                 | 0.2        |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD13 | 7                   | 0.33     | 0.3                 | 0.2        |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB1  | 7                   | 0.3      | 0.13                | 0.28       |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB2  | 7                   | 0.3      | 0.13                | 0.28       |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB3  | 7                   | 0.3      | 0.13                | 0.28       |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB1  | 7                   | 0.3      | 0.13                | 0.28       |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB2  | 7                   | 0.3      | 0.13                | 0.28       |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB3  | 7                   | 0.3      | 0.13                | 0.28       |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB1  | 7                   | 0.3      | 0.13                | 0.28       |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB2  | 7                   | 0.3      | 0.13                | 0.28       |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB3  | 7                   | 0.3      | 0.13                | 0.28       |
| (1,87)   | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD1 | 7                   | 0.21     | 0.09                | 0.22       |
| (1,87)   | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD2 | 7                   | 0.21     | 0.09                | 0.22       |
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD1 | 7                   | 0.21     | 0.09                | 0.22       |
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD2 | 7                   | 0.21     | 0.09                | 0.22       |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD1 | 7                   | 0.21     | 0.09                | 0.22       |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD2 | 7                   | 0.21     | 0.09                | 0.22       |
| (1,2176) | 1:109:A:LEU:HD21 | 1:108:A:SER:HA  | 7                   | 0.19     | 0.04                | 0.2        |
| (1,2176) | 1:109:A:LEU:HD22 | 1:108:A:SER:HA  | 7                   | 0.19     | 0.04                | 0.2        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2176) | 1:109:A:LEU:HD23 | 1:108:A:SER:HA   | 7                   | 0.19     | 0.04                | 0.2        |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB2   | 7                   | 0.13     | 0.03                | 0.11       |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB3   | 7                   | 0.13     | 0.03                | 0.11       |
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB2   | 7                   | 0.13     | 0.03                | 0.11       |
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB3   | 7                   | 0.13     | 0.03                | 0.11       |
| (1,486)  | 1:123:A:VAL:HA   | 1:18:A:ALA:HA    | 7                   | 0.12     | 0.02                | 0.13       |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG11   | 6                   | 1.07     | 0.95                | 1.02       |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG12   | 6                   | 1.07     | 0.95                | 1.02       |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG13   | 6                   | 1.07     | 0.95                | 1.02       |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG11   | 6                   | 1.07     | 0.95                | 1.02       |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG12   | 6                   | 1.07     | 0.95                | 1.02       |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG13   | 6                   | 1.07     | 0.95                | 1.02       |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG11   | 6                   | 1.07     | 0.95                | 1.02       |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG12   | 6                   | 1.07     | 0.95                | 1.02       |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG13   | 6                   | 1.07     | 0.95                | 1.02       |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD11  | 6                   | 0.68     | 0.39                | 0.72       |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD12  | 6                   | 0.68     | 0.39                | 0.72       |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD13  | 6                   | 0.68     | 0.39                | 0.72       |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD11  | 6                   | 0.68     | 0.39                | 0.72       |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD12  | 6                   | 0.68     | 0.39                | 0.72       |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD13  | 6                   | 0.68     | 0.39                | 0.72       |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD11  | 6                   | 0.68     | 0.39                | 0.72       |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD12  | 6                   | 0.68     | 0.39                | 0.72       |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD13  | 6                   | 0.68     | 0.39                | 0.72       |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG21 | 6                   | 0.25     | 0.06                | 0.22       |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG22 | 6                   | 0.25     | 0.06                | 0.22       |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG23 | 6                   | 0.25     | 0.06                | 0.22       |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG21 | 6                   | 0.25     | 0.06                | 0.22       |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG22 | 6                   | 0.25     | 0.06                | 0.22       |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG23 | 6                   | 0.25     | 0.06                | 0.22       |
| (1,1133) | 1:50:A:MET:HG2   | 1:48:A:ALA:HB1   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,1133) | 1:50:A:MET:HG2   | 1:48:A:ALA:HB2   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,1133) | 1:50:A:MET:HG2   | 1:48:A:ALA:HB3   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,1133) | 1:50:A:MET:HG3   | 1:48:A:ALA:HB1   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,1133) | 1:50:A:MET:HG3   | 1:48:A:ALA:HB2   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,1133) | 1:50:A:MET:HG3   | 1:48:A:ALA:HB3   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,2865) | 1:35:A:SER:HA    | 1:8:A:SER:H      | 6                   | 0.1      | 0.0                 | 0.1        |
| (1,1890) | 1:91:A:VAL:HG11  | 1:92:A:THR:HA    | 5                   | 2.06     | 0.02                | 2.05       |
| (1,1890) | 1:91:A:VAL:HG12  | 1:92:A:THR:HA    | 5                   | 2.06     | 0.02                | 2.05       |
| (1,1890) | 1:91:A:VAL:HG13  | 1:92:A:THR:HA    | 5                   | 2.06     | 0.02                | 2.05       |
| (1,3711) | 1:79:A:LEU:HD11  | 1:16:A:GLN:H     | 5                   | 1.67     | 0.07                | 1.7        |
| (1,3711) | 1:79:A:LEU:HD12  | 1:16:A:GLN:H     | 5                   | 1.67     | 0.07                | 1.7        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3711) | 1:79:A:LEU:HD13 | 1:16:A:GLN:H    | 5                   | 1.67     | 0.07                | 1.7        |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG11 | 5                   | 1.63     | 0.04                | 1.61       |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG12 | 5                   | 1.63     | 0.04                | 1.61       |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG13 | 5                   | 1.63     | 0.04                | 1.61       |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG11 | 5                   | 1.63     | 0.04                | 1.61       |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG12 | 5                   | 1.63     | 0.04                | 1.61       |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG13 | 5                   | 1.63     | 0.04                | 1.61       |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG11 | 5                   | 1.63     | 0.04                | 1.61       |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG12 | 5                   | 1.63     | 0.04                | 1.61       |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG13 | 5                   | 1.63     | 0.04                | 1.61       |
| (1,1898) | 1:91:A:VAL:HG11 | 1:92:A:THR:HG21 | 5                   | 0.93     | 0.04                | 0.91       |
| (1,1898) | 1:91:A:VAL:HG11 | 1:92:A:THR:HG22 | 5                   | 0.93     | 0.04                | 0.91       |
| (1,1898) | 1:91:A:VAL:HG11 | 1:92:A:THR:HG23 | 5                   | 0.93     | 0.04                | 0.91       |
| (1,1898) | 1:91:A:VAL:HG12 | 1:92:A:THR:HG21 | 5                   | 0.93     | 0.04                | 0.91       |
| (1,1898) | 1:91:A:VAL:HG12 | 1:92:A:THR:HG22 | 5                   | 0.93     | 0.04                | 0.91       |
| (1,1898) | 1:91:A:VAL:HG12 | 1:92:A:THR:HG23 | 5                   | 0.93     | 0.04                | 0.91       |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG21 | 5                   | 0.93     | 0.04                | 0.91       |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG22 | 5                   | 0.93     | 0.04                | 0.91       |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG23 | 5                   | 0.93     | 0.04                | 0.91       |
| (1,2084) | 1:79:A:LEU:HD21 | 1:101:A:LEU:HG  | 5                   | 0.83     | 0.26                | 0.82       |
| (1,2084) | 1:79:A:LEU:HD22 | 1:101:A:LEU:HG  | 5                   | 0.83     | 0.26                | 0.82       |
| (1,2084) | 1:79:A:LEU:HD23 | 1:101:A:LEU:HG  | 5                   | 0.83     | 0.26                | 0.82       |
| (1,1738) | 1:15:A:SER:HA   | 1:79:A:LEU:HD11 | 5                   | 0.72     | 0.12                | 0.69       |
| (1,1738) | 1:15:A:SER:HA   | 1:79:A:LEU:HD12 | 5                   | 0.72     | 0.12                | 0.69       |
| (1,1738) | 1:15:A:SER:HA   | 1:79:A:LEU:HD13 | 5                   | 0.72     | 0.12                | 0.69       |
| (1,2744) | 1:79:A:LEU:HD11 | 1:15:A:SER:HA   | 5                   | 0.72     | 0.12                | 0.69       |
| (1,2744) | 1:79:A:LEU:HD12 | 1:15:A:SER:HA   | 5                   | 0.72     | 0.12                | 0.69       |
| (1,2744) | 1:79:A:LEU:HD13 | 1:15:A:SER:HA   | 5                   | 0.72     | 0.12                | 0.69       |
| (1,1794) | 1:91:A:VAL:HG21 | 1:86:A:LEU:HG   | 5                   | 0.63     | 0.05                | 0.64       |
| (1,1794) | 1:91:A:VAL:HG22 | 1:86:A:LEU:HG   | 5                   | 0.63     | 0.05                | 0.64       |
| (1,1794) | 1:91:A:VAL:HG23 | 1:86:A:LEU:HG   | 5                   | 0.63     | 0.05                | 0.64       |
| (1,1737) | 1:15:A:SER:HB2  | 1:79:A:LEU:HD11 | 5                   | 0.4      | 0.2                 | 0.29       |
| (1,1737) | 1:15:A:SER:HB2  | 1:79:A:LEU:HD12 | 5                   | 0.4      | 0.2                 | 0.29       |
| (1,1737) | 1:15:A:SER:HB2  | 1:79:A:LEU:HD13 | 5                   | 0.4      | 0.2                 | 0.29       |
| (1,1737) | 1:15:A:SER:HB3  | 1:79:A:LEU:HD11 | 5                   | 0.4      | 0.2                 | 0.29       |
| (1,1737) | 1:15:A:SER:HB3  | 1:79:A:LEU:HD12 | 5                   | 0.4      | 0.2                 | 0.29       |
| (1,1737) | 1:15:A:SER:HB3  | 1:79:A:LEU:HD13 | 5                   | 0.4      | 0.2                 | 0.29       |
| (1,1796) | 1:91:A:VAL:HG21 | 1:86:A:LEU:HD11 | 5                   | 0.38     | 0.08                | 0.36       |
| (1,1796) | 1:91:A:VAL:HG21 | 1:86:A:LEU:HD12 | 5                   | 0.38     | 0.08                | 0.36       |
| (1,1796) | 1:91:A:VAL:HG21 | 1:86:A:LEU:HD13 | 5                   | 0.38     | 0.08                | 0.36       |
| (1,1796) | 1:91:A:VAL:HG22 | 1:86:A:LEU:HD11 | 5                   | 0.38     | 0.08                | 0.36       |
| (1,1796) | 1:91:A:VAL:HG22 | 1:86:A:LEU:HD12 | 5                   | 0.38     | 0.08                | 0.36       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD13 | 5                   | 0.38     | 0.08                | 0.36       |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD11 | 5                   | 0.38     | 0.08                | 0.36       |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD12 | 5                   | 0.38     | 0.08                | 0.36       |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD13 | 5                   | 0.38     | 0.08                | 0.36       |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB2 | 5                   | 0.31     | 0.29                | 0.16       |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB3 | 5                   | 0.31     | 0.29                | 0.16       |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB2 | 5                   | 0.31     | 0.29                | 0.16       |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB3 | 5                   | 0.31     | 0.29                | 0.16       |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB2 | 5                   | 0.31     | 0.29                | 0.16       |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB3 | 5                   | 0.31     | 0.29                | 0.16       |
| (1,2124) | 1:4:A:VAL:HG21   | 1:126:A:LEU:HG  | 5                   | 0.26     | 0.17                | 0.17       |
| (1,2124) | 1:4:A:VAL:HG22   | 1:126:A:LEU:HG  | 5                   | 0.26     | 0.17                | 0.17       |
| (1,2124) | 1:4:A:VAL:HG23   | 1:126:A:LEU:HG  | 5                   | 0.26     | 0.17                | 0.17       |
| (1,262)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG21  | 5                   | 0.2      | 0.08                | 0.26       |
| (1,262)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG22  | 5                   | 0.2      | 0.08                | 0.26       |
| (1,262)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG23  | 5                   | 0.2      | 0.08                | 0.26       |
| (1,262)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG21  | 5                   | 0.2      | 0.08                | 0.26       |
| (1,262)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG22  | 5                   | 0.2      | 0.08                | 0.26       |
| (1,262)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG23  | 5                   | 0.2      | 0.08                | 0.26       |
| (1,262)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG21  | 5                   | 0.2      | 0.08                | 0.26       |
| (1,262)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG22  | 5                   | 0.2      | 0.08                | 0.26       |
| (1,262)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG23  | 5                   | 0.2      | 0.08                | 0.26       |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG11 | 5                   | 0.19     | 0.04                | 0.18       |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG12 | 5                   | 0.19     | 0.04                | 0.18       |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG13 | 5                   | 0.19     | 0.04                | 0.18       |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG11 | 5                   | 0.19     | 0.04                | 0.18       |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG12 | 5                   | 0.19     | 0.04                | 0.18       |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG13 | 5                   | 0.19     | 0.04                | 0.18       |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG11 | 5                   | 0.19     | 0.04                | 0.18       |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG12 | 5                   | 0.19     | 0.04                | 0.18       |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG13 | 5                   | 0.19     | 0.04                | 0.18       |
| (1,318)  | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG21  | 5                   | 0.16     | 0.03                | 0.15       |
| (1,318)  | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG22  | 5                   | 0.16     | 0.03                | 0.15       |
| (1,318)  | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG23  | 5                   | 0.16     | 0.03                | 0.15       |
| (1,318)  | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG21  | 5                   | 0.16     | 0.03                | 0.15       |
| (1,318)  | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG22  | 5                   | 0.16     | 0.03                | 0.15       |
| (1,318)  | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG23  | 5                   | 0.16     | 0.03                | 0.15       |
| (1,318)  | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG21  | 5                   | 0.16     | 0.03                | 0.15       |
| (1,318)  | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG22  | 5                   | 0.16     | 0.03                | 0.15       |
| (1,318)  | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG23  | 5                   | 0.16     | 0.03                | 0.15       |
| (1,340)  | 1:104:A:PRO:HD2  | 1:8:A:SER:HB2   | 5                   | 0.16     | 0.04                | 0.15       |
| (1,340)  | 1:104:A:PRO:HD2  | 1:8:A:SER:HB3   | 5                   | 0.16     | 0.04                | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,340)  | 1:104:A:PRO:HD3 | 1:8:A:SER:HB2   | 5                   | 0.16     | 0.04                | 0.15       |
| (1,340)  | 1:104:A:PRO:HD3 | 1:8:A:SER:HB3   | 5                   | 0.16     | 0.04                | 0.15       |
| (1,1476) | 1:7:A:VAL:HG21  | 1:65:A:ILE:HD11 | 5                   | 0.16     | 0.03                | 0.15       |
| (1,1476) | 1:7:A:VAL:HG21  | 1:65:A:ILE:HD12 | 5                   | 0.16     | 0.03                | 0.15       |
| (1,1476) | 1:7:A:VAL:HG21  | 1:65:A:ILE:HD13 | 5                   | 0.16     | 0.03                | 0.15       |
| (1,1476) | 1:7:A:VAL:HG22  | 1:65:A:ILE:HD11 | 5                   | 0.16     | 0.03                | 0.15       |
| (1,1476) | 1:7:A:VAL:HG22  | 1:65:A:ILE:HD12 | 5                   | 0.16     | 0.03                | 0.15       |
| (1,1476) | 1:7:A:VAL:HG22  | 1:65:A:ILE:HD13 | 5                   | 0.16     | 0.03                | 0.15       |
| (1,1476) | 1:7:A:VAL:HG23  | 1:65:A:ILE:HD11 | 5                   | 0.16     | 0.03                | 0.15       |
| (1,1476) | 1:7:A:VAL:HG23  | 1:65:A:ILE:HD12 | 5                   | 0.16     | 0.03                | 0.15       |
| (1,1476) | 1:7:A:VAL:HG23  | 1:65:A:ILE:HD13 | 5                   | 0.16     | 0.03                | 0.15       |
| (1,1701) | 1:101:A:LEU:HG  | 1:77:A:ILE:HG21 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1701) | 1:101:A:LEU:HG  | 1:77:A:ILE:HG22 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,1701) | 1:101:A:LEU:HG  | 1:77:A:ILE:HG23 | 5                   | 0.13     | 0.01                | 0.13       |
| (1,3033) | 1:112:A:PHE:HB2 | 1:106:A:GLY:H   | 5                   | 0.12     | 0.02                | 0.11       |
| (1,3033) | 1:112:A:PHE:HB3 | 1:106:A:GLY:H   | 5                   | 0.12     | 0.02                | 0.11       |
| (1,3504) | 1:43:A:HIS:HE1  | 1:105:A:ASP:H   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,244)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HB    | 4                   | 1.12     | 0.12                | 1.11       |
| (1,244)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HB    | 4                   | 1.12     | 0.12                | 1.11       |
| (1,244)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HB    | 4                   | 1.12     | 0.12                | 1.11       |
| (1,1684) | 1:4:A:VAL:HG21  | 1:77:A:ILE:HG12 | 4                   | 0.97     | 0.18                | 0.98       |
| (1,1684) | 1:4:A:VAL:HG21  | 1:77:A:ILE:HG13 | 4                   | 0.97     | 0.18                | 0.98       |
| (1,1684) | 1:4:A:VAL:HG22  | 1:77:A:ILE:HG12 | 4                   | 0.97     | 0.18                | 0.98       |
| (1,1684) | 1:4:A:VAL:HG22  | 1:77:A:ILE:HG13 | 4                   | 0.97     | 0.18                | 0.98       |
| (1,1684) | 1:4:A:VAL:HG23  | 1:77:A:ILE:HG12 | 4                   | 0.97     | 0.18                | 0.98       |
| (1,1684) | 1:4:A:VAL:HG23  | 1:77:A:ILE:HG13 | 4                   | 0.97     | 0.18                | 0.98       |
| (1,254)  | 1:99:A:TRP:HH2  | 1:4:A:VAL:HG11  | 4                   | 0.76     | 0.13                | 0.72       |
| (1,254)  | 1:99:A:TRP:HH2  | 1:4:A:VAL:HG12  | 4                   | 0.76     | 0.13                | 0.72       |
| (1,254)  | 1:99:A:TRP:HH2  | 1:4:A:VAL:HG13  | 4                   | 0.76     | 0.13                | 0.72       |
| (1,264)  | 1:75:A:VAL:HG21 | 1:4:A:VAL:HG21  | 4                   | 0.68     | 0.6                 | 0.39       |
| (1,264)  | 1:75:A:VAL:HG21 | 1:4:A:VAL:HG22  | 4                   | 0.68     | 0.6                 | 0.39       |
| (1,264)  | 1:75:A:VAL:HG21 | 1:4:A:VAL:HG23  | 4                   | 0.68     | 0.6                 | 0.39       |
| (1,264)  | 1:75:A:VAL:HG22 | 1:4:A:VAL:HG21  | 4                   | 0.68     | 0.6                 | 0.39       |
| (1,264)  | 1:75:A:VAL:HG22 | 1:4:A:VAL:HG22  | 4                   | 0.68     | 0.6                 | 0.39       |
| (1,264)  | 1:75:A:VAL:HG22 | 1:4:A:VAL:HG23  | 4                   | 0.68     | 0.6                 | 0.39       |
| (1,264)  | 1:75:A:VAL:HG23 | 1:4:A:VAL:HG21  | 4                   | 0.68     | 0.6                 | 0.39       |
| (1,264)  | 1:75:A:VAL:HG23 | 1:4:A:VAL:HG22  | 4                   | 0.68     | 0.6                 | 0.39       |
| (1,264)  | 1:75:A:VAL:HG23 | 1:4:A:VAL:HG23  | 4                   | 0.68     | 0.6                 | 0.39       |
| (1,1216) | 1:53:A:VAL:HG21 | 1:52:A:GLU:HA   | 4                   | 0.63     | 0.04                | 0.64       |
| (1,1216) | 1:53:A:VAL:HG22 | 1:52:A:GLU:HA   | 4                   | 0.63     | 0.04                | 0.64       |
| (1,1216) | 1:53:A:VAL:HG23 | 1:52:A:GLU:HA   | 4                   | 0.63     | 0.04                | 0.64       |
| (1,1664) | 1:79:A:LEU:HD21 | 1:77:A:ILE:HA   | 4                   | 0.63     | 0.07                | 0.63       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1664) | 1:79:A:LEU:HD22  | 1:77:A:ILE:HA    | 4                   | 0.63     | 0.07                | 0.63       |
| (1,1664) | 1:79:A:LEU:HD23  | 1:77:A:ILE:HA    | 4                   | 0.63     | 0.07                | 0.63       |
| (1,3472) | 1:79:A:LEU:HD21  | 1:99:A:TRP:H     | 4                   | 0.49     | 0.16                | 0.56       |
| (1,3472) | 1:79:A:LEU:HD22  | 1:99:A:TRP:H     | 4                   | 0.49     | 0.16                | 0.56       |
| (1,3472) | 1:79:A:LEU:HD23  | 1:99:A:TRP:H     | 4                   | 0.49     | 0.16                | 0.56       |
| (1,1755) | 1:91:A:VAL:HG21  | 1:83:A:GLY:HA2   | 4                   | 0.45     | 0.24                | 0.44       |
| (1,1755) | 1:91:A:VAL:HG21  | 1:83:A:GLY:HA3   | 4                   | 0.45     | 0.24                | 0.44       |
| (1,1755) | 1:91:A:VAL:HG22  | 1:83:A:GLY:HA2   | 4                   | 0.45     | 0.24                | 0.44       |
| (1,1755) | 1:91:A:VAL:HG22  | 1:83:A:GLY:HA3   | 4                   | 0.45     | 0.24                | 0.44       |
| (1,1755) | 1:91:A:VAL:HG23  | 1:83:A:GLY:HA2   | 4                   | 0.45     | 0.24                | 0.44       |
| (1,1755) | 1:91:A:VAL:HG23  | 1:83:A:GLY:HA3   | 4                   | 0.45     | 0.24                | 0.44       |
| (1,2434) | 1:79:A:LEU:HD21  | 1:119:A:VAL:HG21 | 4                   | 0.43     | 0.15                | 0.47       |
| (1,2434) | 1:79:A:LEU:HD21  | 1:119:A:VAL:HG22 | 4                   | 0.43     | 0.15                | 0.47       |
| (1,2434) | 1:79:A:LEU:HD21  | 1:119:A:VAL:HG23 | 4                   | 0.43     | 0.15                | 0.47       |
| (1,2434) | 1:79:A:LEU:HD22  | 1:119:A:VAL:HG21 | 4                   | 0.43     | 0.15                | 0.47       |
| (1,2434) | 1:79:A:LEU:HD22  | 1:119:A:VAL:HG22 | 4                   | 0.43     | 0.15                | 0.47       |
| (1,2434) | 1:79:A:LEU:HD22  | 1:119:A:VAL:HG23 | 4                   | 0.43     | 0.15                | 0.47       |
| (1,2434) | 1:79:A:LEU:HD23  | 1:119:A:VAL:HG21 | 4                   | 0.43     | 0.15                | 0.47       |
| (1,2434) | 1:79:A:LEU:HD23  | 1:119:A:VAL:HG22 | 4                   | 0.43     | 0.15                | 0.47       |
| (1,2434) | 1:79:A:LEU:HD23  | 1:119:A:VAL:HG23 | 4                   | 0.43     | 0.15                | 0.47       |
| (1,1248) | 1:53:A:VAL:H     | 1:53:A:VAL:HG21  | 4                   | 0.4      | 0.03                | 0.4        |
| (1,1248) | 1:53:A:VAL:H     | 1:53:A:VAL:HG22  | 4                   | 0.4      | 0.03                | 0.4        |
| (1,1248) | 1:53:A:VAL:H     | 1:53:A:VAL:HG23  | 4                   | 0.4      | 0.03                | 0.4        |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG11  | 4                   | 0.2      | 0.03                | 0.2        |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG12  | 4                   | 0.2      | 0.03                | 0.2        |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG13  | 4                   | 0.2      | 0.03                | 0.2        |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG11  | 4                   | 0.2      | 0.03                | 0.2        |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG12  | 4                   | 0.2      | 0.03                | 0.2        |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG13  | 4                   | 0.2      | 0.03                | 0.2        |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG11  | 4                   | 0.2      | 0.03                | 0.2        |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG12  | 4                   | 0.2      | 0.03                | 0.2        |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG13  | 4                   | 0.2      | 0.03                | 0.2        |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG21 | 4                   | 0.18     | 0.03                | 0.18       |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG22 | 4                   | 0.18     | 0.03                | 0.18       |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG23 | 4                   | 0.18     | 0.03                | 0.18       |
| (1,3559) | 1:111:A:VAL:HG21 | 1:115:A:VAL:H    | 4                   | 0.18     | 0.03                | 0.18       |
| (1,3559) | 1:111:A:VAL:HG22 | 1:115:A:VAL:H    | 4                   | 0.18     | 0.03                | 0.18       |
| (1,3559) | 1:111:A:VAL:HG23 | 1:115:A:VAL:H    | 4                   | 0.18     | 0.03                | 0.18       |
| (1,2022) | 1:100:A:GLN:H    | 1:98:A:ASP:HA    | 4                   | 0.16     | 0.03                | 0.16       |
| (1,2673) | 1:127:A:ILE:H    | 1:127:A:ILE:HG12 | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,2673) | 1:127:A:ILE:H    | 1:127:A:ILE:HG13 | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,3657) | 1:127:A:ILE:HG12 | 1:127:A:ILE:H    | 4                   | 0.1      | 0.0                 | 0.1        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3657) | 1:127:A:ILE:HG13 | 1:127:A:ILE:H    | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,2083) | 1:119:A:VAL:HG21 | 1:101:A:LEU:HG   | 3                   | 1.9      | 0.1                 | 1.95       |
| (1,2083) | 1:119:A:VAL:HG22 | 1:101:A:LEU:HG   | 3                   | 1.9      | 0.1                 | 1.95       |
| (1,2083) | 1:119:A:VAL:HG23 | 1:101:A:LEU:HG   | 3                   | 1.9      | 0.1                 | 1.95       |
| (1,2769) | 1:4:A:VAL:HG21   | 1:30:A:ILE:HB    | 3                   | 1.27     | 0.15                | 1.24       |
| (1,2769) | 1:4:A:VAL:HG22   | 1:30:A:ILE:HB    | 3                   | 1.27     | 0.15                | 1.24       |
| (1,2769) | 1:4:A:VAL:HG23   | 1:30:A:ILE:HB    | 3                   | 1.27     | 0.15                | 1.24       |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG11 | 3                   | 1.07     | 0.01                | 1.07       |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG12 | 3                   | 1.07     | 0.01                | 1.07       |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG13 | 3                   | 1.07     | 0.01                | 1.07       |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG11 | 3                   | 0.93     | 0.08                | 0.88       |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG12 | 3                   | 0.93     | 0.08                | 0.88       |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG13 | 3                   | 0.93     | 0.08                | 0.88       |
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG11 | 3                   | 0.93     | 0.08                | 0.88       |
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG12 | 3                   | 0.93     | 0.08                | 0.88       |
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG13 | 3                   | 0.93     | 0.08                | 0.88       |
| (1,1240) | 1:116:A:ARG:HG2  | 1:53:A:VAL:HG11  | 3                   | 0.88     | 0.45                | 0.64       |
| (1,1240) | 1:116:A:ARG:HG2  | 1:53:A:VAL:HG12  | 3                   | 0.88     | 0.45                | 0.64       |
| (1,1240) | 1:116:A:ARG:HG2  | 1:53:A:VAL:HG13  | 3                   | 0.88     | 0.45                | 0.64       |
| (1,1240) | 1:116:A:ARG:HG3  | 1:53:A:VAL:HG11  | 3                   | 0.88     | 0.45                | 0.64       |
| (1,1240) | 1:116:A:ARG:HG3  | 1:53:A:VAL:HG12  | 3                   | 0.88     | 0.45                | 0.64       |
| (1,1240) | 1:116:A:ARG:HG3  | 1:53:A:VAL:HG13  | 3                   | 0.88     | 0.45                | 0.64       |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG21 | 3                   | 0.82     | 0.02                | 0.81       |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG22 | 3                   | 0.82     | 0.02                | 0.81       |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG23 | 3                   | 0.82     | 0.02                | 0.81       |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG21 | 3                   | 0.82     | 0.02                | 0.81       |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG22 | 3                   | 0.82     | 0.02                | 0.81       |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG23 | 3                   | 0.82     | 0.02                | 0.81       |
| (1,2357) | 1:119:A:VAL:HG11 | 1:116:A:ARG:HG2  | 3                   | 0.41     | 0.02                | 0.4        |
| (1,2357) | 1:119:A:VAL:HG11 | 1:116:A:ARG:HG3  | 3                   | 0.41     | 0.02                | 0.4        |
| (1,2357) | 1:119:A:VAL:HG12 | 1:116:A:ARG:HG2  | 3                   | 0.41     | 0.02                | 0.4        |
| (1,2357) | 1:119:A:VAL:HG12 | 1:116:A:ARG:HG3  | 3                   | 0.41     | 0.02                | 0.4        |
| (1,2357) | 1:119:A:VAL:HG13 | 1:116:A:ARG:HG2  | 3                   | 0.41     | 0.02                | 0.4        |
| (1,2357) | 1:119:A:VAL:HG13 | 1:116:A:ARG:HG3  | 3                   | 0.41     | 0.02                | 0.4        |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG11 | 3                   | 0.32     | 0.14                | 0.23       |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG12 | 3                   | 0.32     | 0.14                | 0.23       |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG13 | 3                   | 0.32     | 0.14                | 0.23       |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG11 | 3                   | 0.32     | 0.14                | 0.23       |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG12 | 3                   | 0.32     | 0.14                | 0.23       |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG13 | 3                   | 0.32     | 0.14                | 0.23       |
| (1,2405) | 1:119:A:VAL:H    | 1:119:A:VAL:HB   | 3                   | 0.17     | 0.0                 | 0.17       |
| (1,2408) | 1:116:A:ARG:HA   | 1:119:A:VAL:HB   | 3                   | 0.15     | 0.01                | 0.15       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1980) | 1:91:A:VAL:H     | 1:96:A:PHE:HB2  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1980) | 1:91:A:VAL:H     | 1:96:A:PHE:HB3  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,802)  | 1:33:A:THR:HA    | 1:32:A:VAL:HG11 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,802)  | 1:33:A:THR:HA    | 1:32:A:VAL:HG12 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,802)  | 1:33:A:THR:HA    | 1:32:A:VAL:HG13 | 3                   | 0.11     | 0.01                | 0.11       |
| (1,3666) | 1:130:A:ILE:HD11 | 1:128:A:ALA:H   | 3                   | 0.11     | 0.01                | 0.12       |
| (1,3666) | 1:130:A:ILE:HD12 | 1:128:A:ALA:H   | 3                   | 0.11     | 0.01                | 0.12       |
| (1,3666) | 1:130:A:ILE:HD13 | 1:128:A:ALA:H   | 3                   | 0.11     | 0.01                | 0.12       |
| (1,1253) | 1:24:A:THR:HB    | 1:54:A:GLY:HA2  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,1253) | 1:24:A:THR:HB    | 1:54:A:GLY:HA3  | 3                   | 0.11     | 0.01                | 0.11       |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB1 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB2 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB3 | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,2546) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HA  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,2546) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HA  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG21 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG22 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG23 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG21 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG22 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG23 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG21 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG22 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG23 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG21 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG22 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG23 | 2                   | 0.47     | 0.03                | 0.47       |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD21 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD22 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD21 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD22 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD21 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD22 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD21 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD22 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD21 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD22 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD21 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD22 | 2                   | 0.33     | 0.11                | 0.33       |
| (1,1456) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HB   | 2                   | 0.23     | 0.09                | 0.23       |
| (1,1456) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HB   | 2                   | 0.23     | 0.09                | 0.23       |
| (1,1456) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HB   | 2                   | 0.23     | 0.09                | 0.23       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1734) | 1:119:A:VAL:HG21 | 1:79:A:LEU:HD11  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1734) | 1:119:A:VAL:HG21 | 1:79:A:LEU:HD12  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1734) | 1:119:A:VAL:HG21 | 1:79:A:LEU:HD13  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1734) | 1:119:A:VAL:HG22 | 1:79:A:LEU:HD11  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1734) | 1:119:A:VAL:HG22 | 1:79:A:LEU:HD12  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1734) | 1:119:A:VAL:HG22 | 1:79:A:LEU:HD13  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1734) | 1:119:A:VAL:HG23 | 1:79:A:LEU:HD11  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1734) | 1:119:A:VAL:HG23 | 1:79:A:LEU:HD12  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1734) | 1:119:A:VAL:HG23 | 1:79:A:LEU:HD13  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,2246) | 1:114:A:THR:HG21 | 1:111:A:VAL:HG21 | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2246) | 1:114:A:THR:HG21 | 1:111:A:VAL:HG22 | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2246) | 1:114:A:THR:HG21 | 1:111:A:VAL:HG23 | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2246) | 1:114:A:THR:HG22 | 1:111:A:VAL:HG21 | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2246) | 1:114:A:THR:HG22 | 1:111:A:VAL:HG22 | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2246) | 1:114:A:THR:HG22 | 1:111:A:VAL:HG23 | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2246) | 1:114:A:THR:HG23 | 1:111:A:VAL:HG21 | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2246) | 1:114:A:THR:HG23 | 1:111:A:VAL:HG22 | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2246) | 1:114:A:THR:HG23 | 1:111:A:VAL:HG23 | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2351) | 1:114:A:THR:H    | 1:116:A:ARG:HG2  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,2351) | 1:114:A:THR:H    | 1:116:A:ARG:HG3  | 2                   | 0.18     | 0.0                 | 0.18       |
| (1,446)  | 1:62:A:SER:HA    | 1:16:A:GLN:HB2   | 2                   | 0.16     | 0.04                | 0.16       |
| (1,446)  | 1:62:A:SER:HA    | 1:16:A:GLN:HB3   | 2                   | 0.16     | 0.04                | 0.16       |
| (1,108)  | 1:90:A:TRP:H     | 1:90:A:TRP:HD1   | 2                   | 0.15     | 0.01                | 0.15       |
| (1,263)  | 1:77:A:ILE:HG12  | 1:4:A:VAL:HG21   | 2                   | 0.15     | 0.02                | 0.15       |
| (1,263)  | 1:77:A:ILE:HG12  | 1:4:A:VAL:HG22   | 2                   | 0.15     | 0.02                | 0.15       |
| (1,263)  | 1:77:A:ILE:HG12  | 1:4:A:VAL:HG23   | 2                   | 0.15     | 0.02                | 0.15       |
| (1,263)  | 1:77:A:ILE:HG13  | 1:4:A:VAL:HG21   | 2                   | 0.15     | 0.02                | 0.15       |
| (1,263)  | 1:77:A:ILE:HG13  | 1:4:A:VAL:HG22   | 2                   | 0.15     | 0.02                | 0.15       |
| (1,263)  | 1:77:A:ILE:HG13  | 1:4:A:VAL:HG23   | 2                   | 0.15     | 0.02                | 0.15       |
| (1,2772) | 1:4:A:VAL:HG21   | 1:77:A:ILE:HG12  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,2772) | 1:4:A:VAL:HG21   | 1:77:A:ILE:HG13  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,2772) | 1:4:A:VAL:HG22   | 1:77:A:ILE:HG12  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,2772) | 1:4:A:VAL:HG22   | 1:77:A:ILE:HG13  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,2772) | 1:4:A:VAL:HG23   | 1:77:A:ILE:HG12  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,2772) | 1:4:A:VAL:HG23   | 1:77:A:ILE:HG13  | 2                   | 0.15     | 0.02                | 0.15       |
| (1,51)   | 1:23:A:LYS:HB2   | 1:25:A:LEU:H     | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,51)   | 1:23:A:LYS:HB3   | 1:25:A:LEU:H     | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1741) | 1:18:A:ALA:H     | 1:79:A:LEU:HD11  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1741) | 1:18:A:ALA:H     | 1:79:A:LEU:HD12  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1741) | 1:18:A:ALA:H     | 1:79:A:LEU:HD13  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,2939) | 1:60:A:GLN:HE21  | 1:22:A:ALA:H     | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2939) | 1:60:A:GLN:HE22  | 1:22:A:ALA:H     | 2                   | 0.12     | 0.02                | 0.12       |

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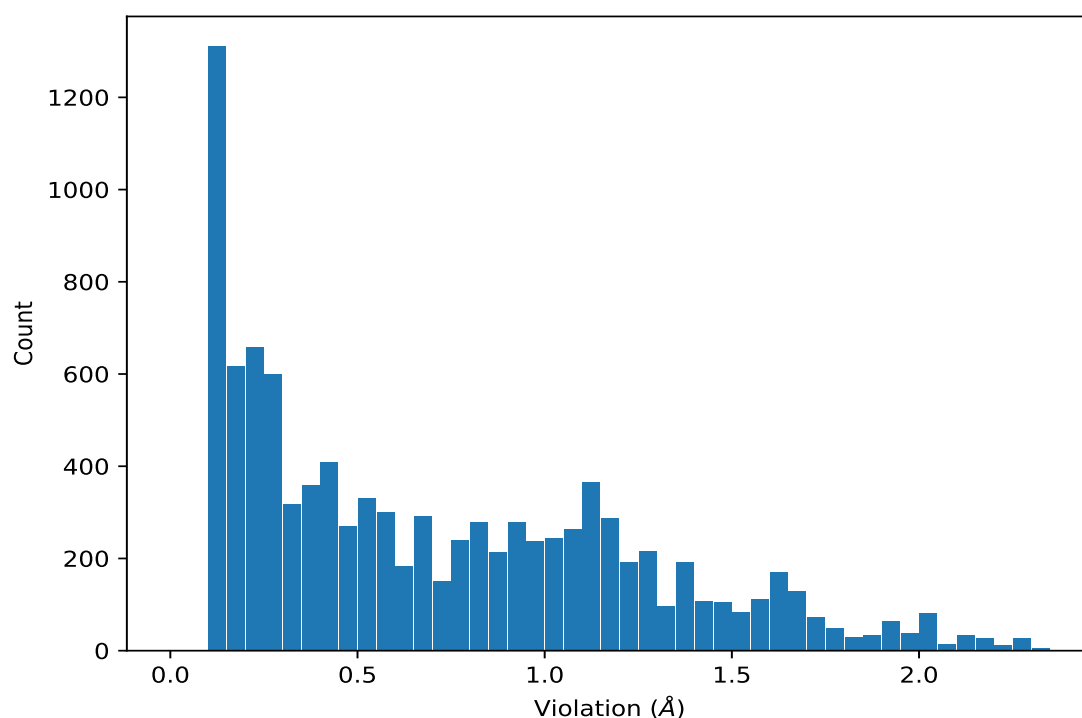
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1340) | 1:41:A:ARG:HG2  | 1:57:A:ILE:HD11 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1340) | 1:41:A:ARG:HG2  | 1:57:A:ILE:HD12 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1340) | 1:41:A:ARG:HG2  | 1:57:A:ILE:HD13 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1340) | 1:41:A:ARG:HG3  | 1:57:A:ILE:HD11 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1340) | 1:41:A:ARG:HG3  | 1:57:A:ILE:HD12 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1340) | 1:41:A:ARG:HG3  | 1:57:A:ILE:HD13 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,2745) | 1:79:A:LEU:HG   | 1:15:A:SER:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2144) | 1:10:A:ARG:HB2  | 1:104:A:PRO:HD2 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,2144) | 1:10:A:ARG:HB2  | 1:104:A:PRO:HD3 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,2144) | 1:10:A:ARG:HB3  | 1:104:A:PRO:HD2 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,2144) | 1:10:A:ARG:HB3  | 1:104:A:PRO:HD3 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,849)  | 1:6:A:PHE:HE1   | 1:34:A:SER:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,849)  | 1:6:A:PHE:HE2   | 1:34:A:SER:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2088) | 1:100:A:GLN:HG2 | 1:101:A:LEU:HG  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,2088) | 1:100:A:GLN:HG3 | 1:101:A:LEU:HG  | 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) |
|----------|-----------------|------------------|----------|---------------|
| (1,2411) | 1:97:A:GLU:HG2  | 1:126:A:LEU:HD11 | 2        | 2.31          |
| (1,2411) | 1:97:A:GLU:HG2  | 1:126:A:LEU:HD12 | 2        | 2.31          |
| (1,2411) | 1:97:A:GLU:HG2  | 1:126:A:LEU:HD13 | 2        | 2.31          |
| (1,2411) | 1:97:A:GLU:HG3  | 1:126:A:LEU:HD11 | 2        | 2.31          |
| (1,2411) | 1:97:A:GLU:HG3  | 1:126:A:LEU:HD12 | 2        | 2.31          |
| (1,2411) | 1:97:A:GLU:HG3  | 1:126:A:LEU:HD13 | 2        | 2.31          |
| (1,3695) | 1:79:A:LEU:HD21 | 1:99:A:TRP:HE1   | 10       | 2.29          |
| (1,3695) | 1:79:A:LEU:HD22 | 1:99:A:TRP:HE1   | 10       | 2.29          |
| (1,3695) | 1:79:A:LEU:HD23 | 1:99:A:TRP:HE1   | 10       | 2.29          |
| (1,2411) | 1:97:A:GLU:HG2  | 1:126:A:LEU:HD11 | 1        | 2.28          |
| (1,2411) | 1:97:A:GLU:HG2  | 1:126:A:LEU:HD12 | 1        | 2.28          |
| (1,2411) | 1:97:A:GLU:HG2  | 1:126:A:LEU:HD13 | 1        | 2.28          |
| (1,2411) | 1:97:A:GLU:HG3  | 1:126:A:LEU:HD11 | 1        | 2.28          |
| (1,2411) | 1:97:A:GLU:HG3  | 1:126:A:LEU:HD12 | 1        | 2.28          |
| (1,2411) | 1:97:A:GLU:HG3  | 1:126:A:LEU:HD13 | 1        | 2.28          |
| (1,2411) | 1:97:A:GLU:HG2  | 1:126:A:LEU:HD11 | 5        | 2.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 5        | 2.28          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 5        | 2.28          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 5        | 2.28          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 5        | 2.28          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 5        | 2.28          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 3        | 2.27          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 3        | 2.27          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 3        | 2.27          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 3        | 2.27          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 3        | 2.27          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 3        | 2.27          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 17       | 2.26          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 17       | 2.26          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 17       | 2.26          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 17       | 2.26          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 17       | 2.26          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 17       | 2.26          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1   | 18       | 2.24          |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1   | 18       | 2.24          |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1   | 18       | 2.24          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 8        | 2.21          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 8        | 2.21          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 8        | 2.21          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 8        | 2.21          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 8        | 2.21          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 8        | 2.21          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 9        | 2.2           |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 9        | 2.2           |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 9        | 2.2           |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 1        | 2.19          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 1        | 2.19          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 1        | 2.19          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 1        | 2.19          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 1        | 2.19          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 1        | 2.19          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1   | 15       | 2.18          |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1   | 15       | 2.18          |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1   | 15       | 2.18          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 13       | 2.18          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 13       | 2.18          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 13       | 2.18          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 13       | 2.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 13       | 2.18          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 13       | 2.18          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 3        | 2.18          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 3        | 2.18          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 3        | 2.18          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 3        | 2.18          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 3        | 2.18          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 3        | 2.18          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 11       | 2.15          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 11       | 2.15          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 11       | 2.15          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 11       | 2.15          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 11       | 2.15          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 11       | 2.15          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1   | 8        | 2.14          |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1   | 8        | 2.14          |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1   | 8        | 2.14          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 20       | 2.14          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 20       | 2.14          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 20       | 2.14          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 20       | 2.14          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 20       | 2.14          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 20       | 2.14          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 16       | 2.12          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 16       | 2.12          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 16       | 2.12          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 16       | 2.12          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 16       | 2.12          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 16       | 2.12          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 20       | 2.12          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 20       | 2.12          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 20       | 2.12          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 20       | 2.12          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 20       | 2.12          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 20       | 2.12          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 19       | 2.11          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 19       | 2.11          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 19       | 2.11          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 19       | 2.11          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 19       | 2.11          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 19       | 2.11          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 18       | 2.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 18       | 2.1           |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 18       | 2.1           |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 18       | 2.1           |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 18       | 2.1           |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 18       | 2.1           |
| (1,1890) | 1:91:A:VAL:HG11  | 1:92:A:THR:HA    | 10       | 2.09          |
| (1,1890) | 1:91:A:VAL:HG12  | 1:92:A:THR:HA    | 10       | 2.09          |
| (1,1890) | 1:91:A:VAL:HG13  | 1:92:A:THR:HA    | 10       | 2.09          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG11   | 17       | 2.08          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG12   | 17       | 2.08          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG13   | 17       | 2.08          |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG11   | 17       | 2.08          |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG12   | 17       | 2.08          |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG13   | 17       | 2.08          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG11   | 17       | 2.08          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG12   | 17       | 2.08          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG13   | 17       | 2.08          |
| (1,1890) | 1:91:A:VAL:HG11  | 1:92:A:THR:HA    | 11       | 2.07          |
| (1,1890) | 1:91:A:VAL:HG12  | 1:92:A:THR:HA    | 11       | 2.07          |
| (1,1890) | 1:91:A:VAL:HG13  | 1:92:A:THR:HA    | 11       | 2.07          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 4        | 2.05          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 4        | 2.05          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 4        | 2.05          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 10       | 2.05          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 10       | 2.05          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 10       | 2.05          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 10       | 2.05          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 10       | 2.05          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 10       | 2.05          |
| (1,1890) | 1:91:A:VAL:HG11  | 1:92:A:THR:HA    | 8        | 2.05          |
| (1,1890) | 1:91:A:VAL:HG12  | 1:92:A:THR:HA    | 8        | 2.05          |
| (1,1890) | 1:91:A:VAL:HG13  | 1:92:A:THR:HA    | 8        | 2.05          |
| (1,1890) | 1:91:A:VAL:HG11  | 1:92:A:THR:HA    | 9        | 2.05          |
| (1,1890) | 1:91:A:VAL:HG12  | 1:92:A:THR:HA    | 9        | 2.05          |
| (1,1890) | 1:91:A:VAL:HG13  | 1:92:A:THR:HA    | 9        | 2.05          |
| (1,1890) | 1:91:A:VAL:HG11  | 1:92:A:THR:HA    | 16       | 2.05          |
| (1,1890) | 1:91:A:VAL:HG12  | 1:92:A:THR:HA    | 16       | 2.05          |
| (1,1890) | 1:91:A:VAL:HG13  | 1:92:A:THR:HA    | 16       | 2.05          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG11   | 7        | 2.05          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG12   | 7        | 2.05          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG13   | 7        | 2.05          |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG11   | 7        | 2.05          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG12   | 7        | 2.05          |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG13   | 7        | 2.05          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG11   | 7        | 2.05          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG12   | 7        | 2.05          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG13   | 7        | 2.05          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 18       | 2.04          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 18       | 2.04          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 18       | 2.04          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11  | 16       | 2.03          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12  | 16       | 2.03          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13  | 16       | 2.03          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 17       | 2.03          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 17       | 2.03          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 17       | 2.03          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 17       | 2.03          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 17       | 2.03          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 17       | 2.03          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 14       | 2.01          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 14       | 2.01          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 14       | 2.01          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 4        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 4        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 4        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 4        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 4        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 4        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 6        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 6        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 6        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 6        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 6        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 6        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 9        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 9        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 9        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 9        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 9        | 2.01          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 9        | 2.01          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 2        | 2.0           |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 2        | 2.0           |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 2        | 2.0           |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 3        | 2.0           |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA | 3        | 2.0           |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA | 3        | 2.0           |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA | 8        | 2.0           |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA | 8        | 2.0           |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA | 8        | 2.0           |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA | 12       | 2.0           |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA | 12       | 2.0           |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA | 12       | 2.0           |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21 | 7        | 2.0           |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22 | 7        | 2.0           |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23 | 7        | 2.0           |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21 | 7        | 2.0           |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22 | 7        | 2.0           |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23 | 7        | 2.0           |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21 | 7        | 2.0           |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22 | 7        | 2.0           |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23 | 7        | 2.0           |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA | 19       | 1.99          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA | 19       | 1.99          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA | 19       | 1.99          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11 | 18       | 1.99          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12 | 18       | 1.99          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13 | 18       | 1.99          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA | 6        | 1.98          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA | 6        | 1.98          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA | 6        | 1.98          |
| (1,2083) | 1:119:A:VAL:HG21 | 1:101:A:LEU:HG | 20       | 1.98          |
| (1,2083) | 1:119:A:VAL:HG22 | 1:101:A:LEU:HG | 20       | 1.98          |
| (1,2083) | 1:119:A:VAL:HG23 | 1:101:A:LEU:HG | 20       | 1.98          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11 | 2        | 1.98          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12 | 2        | 1.98          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13 | 2        | 1.98          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11 | 3        | 1.98          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12 | 3        | 1.98          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13 | 3        | 1.98          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11 | 10       | 1.98          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12 | 10       | 1.98          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13 | 10       | 1.98          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11 | 5        | 1.97          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12 | 5        | 1.97          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13 | 5        | 1.97          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11 | 15       | 1.97          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12   | 15       | 1.97          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13   | 15       | 1.97          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 19       | 1.96          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 19       | 1.96          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 19       | 1.96          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 19       | 1.96          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 19       | 1.96          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 19       | 1.96          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 2        | 1.96          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 2        | 1.96          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 2        | 1.96          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 2        | 1.96          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 2        | 1.96          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 2        | 1.96          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 6        | 1.95          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 6        | 1.95          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 6        | 1.95          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 6        | 1.95          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 6        | 1.95          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 6        | 1.95          |
| (1,2083) | 1:119:A:VAL:HG21 | 1:101:A:LEU:HG   | 1        | 1.95          |
| (1,2083) | 1:119:A:VAL:HG22 | 1:101:A:LEU:HG   | 1        | 1.95          |
| (1,2083) | 1:119:A:VAL:HG23 | 1:101:A:LEU:HG   | 1        | 1.95          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11  | 3        | 1.95          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12  | 3        | 1.95          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13  | 3        | 1.95          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11  | 3        | 1.95          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12  | 3        | 1.95          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13  | 3        | 1.95          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11   | 12       | 1.95          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12   | 12       | 1.95          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13   | 12       | 1.95          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11   | 14       | 1.95          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12   | 14       | 1.95          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13   | 14       | 1.95          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11   | 20       | 1.95          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12   | 20       | 1.95          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13   | 20       | 1.95          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 1        | 1.94          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 1        | 1.94          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 1        | 1.94          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 5        | 1.94          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 5        | 1.94          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 5        | 1.94          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11   | 16       | 1.94          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12   | 16       | 1.94          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13   | 16       | 1.94          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11   | 19       | 1.93          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12   | 19       | 1.93          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13   | 19       | 1.93          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 14       | 1.92          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 14       | 1.92          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 14       | 1.92          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 14       | 1.92          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 14       | 1.92          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 14       | 1.92          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG11   | 13       | 1.92          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG12   | 13       | 1.92          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG13   | 13       | 1.92          |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG11   | 13       | 1.92          |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG12   | 13       | 1.92          |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG13   | 13       | 1.92          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG11   | 13       | 1.92          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG12   | 13       | 1.92          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG13   | 13       | 1.92          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11   | 9        | 1.92          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12   | 9        | 1.92          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13   | 9        | 1.92          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 17       | 1.91          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 17       | 1.91          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 17       | 1.91          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 20       | 1.91          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 20       | 1.91          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 20       | 1.91          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11   | 8        | 1.91          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12   | 8        | 1.91          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13   | 8        | 1.91          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 15       | 1.9           |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 15       | 1.9           |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 15       | 1.9           |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 15       | 1.9           |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 15       | 1.9           |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 15       | 1.9           |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11   | 1        | 1.9           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12   | 1        | 1.9           |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13   | 1        | 1.9           |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11  | 13       | 1.89          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12  | 13       | 1.89          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13  | 13       | 1.89          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11   | 4        | 1.89          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12   | 4        | 1.89          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13   | 4        | 1.89          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11   | 11       | 1.89          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12   | 11       | 1.89          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13   | 11       | 1.89          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 17       | 1.88          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 17       | 1.88          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 17       | 1.88          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 17       | 1.88          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 17       | 1.88          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 17       | 1.88          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 5        | 1.87          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 5        | 1.87          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 5        | 1.87          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 5        | 1.87          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 5        | 1.87          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 5        | 1.87          |
| (1,845)  | 1:79:A:LEU:HD11  | 1:34:A:SER:HA    | 16       | 1.85          |
| (1,845)  | 1:79:A:LEU:HD12  | 1:34:A:SER:HA    | 16       | 1.85          |
| (1,845)  | 1:79:A:LEU:HD13  | 1:34:A:SER:HA    | 16       | 1.85          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 16       | 1.82          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 16       | 1.82          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 16       | 1.82          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 16       | 1.82          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 16       | 1.82          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 16       | 1.82          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 10       | 1.82          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 10       | 1.82          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 10       | 1.82          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 17       | 1.82          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 17       | 1.82          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 17       | 1.82          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 17       | 1.82          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 17       | 1.82          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 17       | 1.82          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 17       | 1.82          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 17       | 1.82          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 17       | 1.82          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 10       | 1.81          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 10       | 1.81          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 10       | 1.81          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 10       | 1.81          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 10       | 1.81          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 10       | 1.81          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 8        | 1.81          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 8        | 1.81          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 8        | 1.81          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 10       | 1.8           |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 10       | 1.8           |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 10       | 1.8           |
| (1,2766) | 1:76:A:VAL:HB    | 1:86:A:LEU:HD11  | 17       | 1.79          |
| (1,2766) | 1:76:A:VAL:HB    | 1:86:A:LEU:HD12  | 17       | 1.79          |
| (1,2766) | 1:76:A:VAL:HB    | 1:86:A:LEU:HD13  | 17       | 1.79          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 1        | 1.78          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 1        | 1.78          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 1        | 1.78          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 12       | 1.77          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 12       | 1.77          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 12       | 1.77          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 12       | 1.77          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 12       | 1.77          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 12       | 1.77          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 15       | 1.77          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 15       | 1.77          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 15       | 1.77          |
| (1,3711) | 1:79:A:LEU:HD11  | 1:16:A:GLN:H     | 16       | 1.76          |
| (1,3711) | 1:79:A:LEU:HD12  | 1:16:A:GLN:H     | 16       | 1.76          |
| (1,3711) | 1:79:A:LEU:HD13  | 1:16:A:GLN:H     | 16       | 1.76          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 8        | 1.76          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 8        | 1.76          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 8        | 1.76          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 8        | 1.76          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 8        | 1.76          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 8        | 1.76          |
| (1,2083) | 1:119:A:VAL:HG21 | 1:101:A:LEU:HG   | 19       | 1.76          |
| (1,2083) | 1:119:A:VAL:HG22 | 1:101:A:LEU:HG   | 19       | 1.76          |
| (1,2083) | 1:119:A:VAL:HG23 | 1:101:A:LEU:HG   | 19       | 1.76          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 9        | 1.75          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 9        | 1.75          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 9        | 1.75          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 9        | 1.75          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 9        | 1.75          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 9        | 1.75          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 9        | 1.75          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 9        | 1.75          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 9        | 1.75          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 17       | 1.75          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 17       | 1.75          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 17       | 1.75          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 17       | 1.75          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 17       | 1.75          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 17       | 1.75          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 17       | 1.75          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 17       | 1.75          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 17       | 1.75          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 17       | 1.75          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 17       | 1.75          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 17       | 1.75          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 13       | 1.74          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 13       | 1.74          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 13       | 1.74          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 19       | 1.74          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 19       | 1.74          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 19       | 1.74          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 9        | 1.73          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 9        | 1.73          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 9        | 1.73          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 9        | 1.73          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 9        | 1.73          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 9        | 1.73          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 19       | 1.73          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 19       | 1.73          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 19       | 1.73          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 16       | 1.73          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 16       | 1.73          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 16       | 1.73          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 7        | 1.73          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 7        | 1.73          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 7        | 1.73          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11   | 7        | 1.73          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12  | 7        | 1.73          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13  | 7        | 1.73          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11  | 7        | 1.73          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12  | 7        | 1.73          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13  | 7        | 1.73          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA   | 17       | 1.73          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA   | 17       | 1.73          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA   | 17       | 1.73          |
| (1,3711) | 1:79:A:LEU:HD11  | 1:16:A:GLN:H    | 10       | 1.72          |
| (1,3711) | 1:79:A:LEU:HD12  | 1:16:A:GLN:H    | 10       | 1.72          |
| (1,3711) | 1:79:A:LEU:HD13  | 1:16:A:GLN:H    | 10       | 1.72          |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H    | 17       | 1.72          |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H    | 17       | 1.72          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H    | 17       | 1.72          |
| (1,1885) | 1:92:A:THR:HG21  | 1:91:A:VAL:HG11 | 10       | 1.72          |
| (1,1885) | 1:92:A:THR:HG21  | 1:91:A:VAL:HG12 | 10       | 1.72          |
| (1,1885) | 1:92:A:THR:HG21  | 1:91:A:VAL:HG13 | 10       | 1.72          |
| (1,1885) | 1:92:A:THR:HG22  | 1:91:A:VAL:HG11 | 10       | 1.72          |
| (1,1885) | 1:92:A:THR:HG22  | 1:91:A:VAL:HG12 | 10       | 1.72          |
| (1,1885) | 1:92:A:THR:HG22  | 1:91:A:VAL:HG13 | 10       | 1.72          |
| (1,1885) | 1:92:A:THR:HG23  | 1:91:A:VAL:HG11 | 10       | 1.72          |
| (1,1885) | 1:92:A:THR:HG23  | 1:91:A:VAL:HG12 | 10       | 1.72          |
| (1,1885) | 1:92:A:THR:HG23  | 1:91:A:VAL:HG13 | 10       | 1.72          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11 | 17       | 1.72          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12 | 17       | 1.72          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13 | 17       | 1.72          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21  | 16       | 1.72          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22  | 16       | 1.72          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23  | 16       | 1.72          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21  | 16       | 1.72          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22  | 16       | 1.72          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23  | 16       | 1.72          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21  | 16       | 1.72          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22  | 16       | 1.72          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23  | 16       | 1.72          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21 | 7        | 1.71          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22 | 7        | 1.71          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23 | 7        | 1.71          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21 | 18       | 1.71          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22 | 18       | 1.71          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23 | 18       | 1.71          |
| (1,264)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG21  | 6        | 1.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,264)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG22   | 6        | 1.71          |
| (1,264)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG23   | 6        | 1.71          |
| (1,264)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG21   | 6        | 1.71          |
| (1,264)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG22   | 6        | 1.71          |
| (1,264)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG23   | 6        | 1.71          |
| (1,264)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG21   | 6        | 1.71          |
| (1,264)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG22   | 6        | 1.71          |
| (1,264)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG23   | 6        | 1.71          |
| (1,3711) | 1:79:A:LEU:HD11  | 1:16:A:GLN:H     | 8        | 1.7           |
| (1,3711) | 1:79:A:LEU:HD12  | 1:16:A:GLN:H     | 8        | 1.7           |
| (1,3711) | 1:79:A:LEU:HD13  | 1:16:A:GLN:H     | 8        | 1.7           |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 20       | 1.7           |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 20       | 1.7           |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 20       | 1.7           |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 20       | 1.7           |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 20       | 1.7           |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 20       | 1.7           |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 20       | 1.7           |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 20       | 1.7           |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 20       | 1.7           |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 20       | 1.7           |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 20       | 1.7           |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 20       | 1.7           |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 7        | 1.7           |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 7        | 1.7           |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 7        | 1.7           |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 7        | 1.7           |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 7        | 1.7           |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 7        | 1.7           |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 2        | 1.7           |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 2        | 1.7           |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 2        | 1.7           |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 3        | 1.7           |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 3        | 1.7           |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 3        | 1.7           |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 7        | 1.69          |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 7        | 1.69          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 7        | 1.69          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 7        | 1.69          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 7        | 1.69          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 7        | 1.69          |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 3        | 1.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 3        | 1.68          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 3        | 1.68          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 2        | 1.68          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 2        | 1.68          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 2        | 1.68          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 2        | 1.68          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 2        | 1.68          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 2        | 1.68          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 11       | 1.68          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 11       | 1.68          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 11       | 1.68          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 11       | 1.68          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 11       | 1.68          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 11       | 1.68          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 16       | 1.68          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 16       | 1.68          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 16       | 1.68          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 16       | 1.68          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 16       | 1.68          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 16       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 2        | 1.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 2        | 1.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 2        | 1.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 2        | 1.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 2        | 1.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 2        | 1.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 11       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 11       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 11       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 11       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 11       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 11       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 16       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 16       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 16       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 16       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 16       | 1.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 16       | 1.68          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 9        | 1.68          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 9        | 1.68          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 9        | 1.68          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 19       | 1.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 19       | 1.68          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 19       | 1.68          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 19       | 1.68          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 19       | 1.68          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 19       | 1.68          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 3        | 1.68          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 3        | 1.68          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 3        | 1.68          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2   | 13       | 1.68          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3   | 13       | 1.68          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2   | 13       | 1.68          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3   | 13       | 1.68          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2   | 13       | 1.68          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3   | 13       | 1.68          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 11       | 1.67          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 11       | 1.67          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 11       | 1.67          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 11       | 1.67          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 11       | 1.67          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 11       | 1.67          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 13       | 1.67          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 13       | 1.67          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 13       | 1.67          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 15       | 1.67          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 15       | 1.67          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 15       | 1.67          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 15       | 1.67          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 15       | 1.67          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 15       | 1.67          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 15       | 1.67          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 15       | 1.67          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 15       | 1.67          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 15       | 1.67          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 15       | 1.67          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 15       | 1.67          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 5        | 1.66          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 5        | 1.66          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 5        | 1.66          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 5        | 1.66          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 5        | 1.66          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 5        | 1.66          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 5        | 1.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 5        | 1.66          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 5        | 1.66          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 5        | 1.66          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 5        | 1.66          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 5        | 1.66          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD11 | 7        | 1.66          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD12 | 7        | 1.66          |
| (1,2411) | 1:97:A:GLU:HG2   | 1:126:A:LEU:HD13 | 7        | 1.66          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD11 | 7        | 1.66          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD12 | 7        | 1.66          |
| (1,2411) | 1:97:A:GLU:HG3   | 1:126:A:LEU:HD13 | 7        | 1.66          |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 12       | 1.65          |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 12       | 1.65          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 12       | 1.65          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 1        | 1.65          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 1        | 1.65          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 1        | 1.65          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 1        | 1.65          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 1        | 1.65          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 1        | 1.65          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 1        | 1.65          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 1        | 1.65          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 1        | 1.65          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 1        | 1.65          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 1        | 1.65          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 1        | 1.65          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 9        | 1.65          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 9        | 1.65          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 9        | 1.65          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 9        | 1.65          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 9        | 1.65          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 9        | 1.65          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 4        | 1.65          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 4        | 1.65          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 4        | 1.65          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 4        | 1.65          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 4        | 1.65          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 4        | 1.65          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 12       | 1.65          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 12       | 1.65          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 12       | 1.65          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 11       | 1.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 11       | 1.64          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 11       | 1.64          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 14       | 1.64          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 14       | 1.64          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 14       | 1.64          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 13       | 1.64          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 13       | 1.64          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 13       | 1.64          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11   | 13       | 1.64          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12   | 13       | 1.64          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13   | 13       | 1.64          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11   | 13       | 1.64          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12   | 13       | 1.64          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13   | 13       | 1.64          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 13       | 1.63          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 13       | 1.63          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 13       | 1.63          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 6        | 1.63          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 6        | 1.63          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 6        | 1.63          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 7        | 1.62          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 7        | 1.62          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 7        | 1.62          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 7        | 1.62          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 7        | 1.62          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 7        | 1.62          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 7        | 1.62          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 7        | 1.62          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 7        | 1.62          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 7        | 1.62          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 7        | 1.62          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 7        | 1.62          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 13       | 1.62          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 13       | 1.62          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 13       | 1.62          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 13       | 1.62          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 13       | 1.62          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 13       | 1.62          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 19       | 1.62          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 19       | 1.62          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 19       | 1.62          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 19       | 1.62          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2431) | 1:122:A:ARG:HD3 | 1:119:A:VAL:HG22 | 19       | 1.62          |
| (1,2431) | 1:122:A:ARG:HD3 | 1:119:A:VAL:HG23 | 19       | 1.62          |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG11  | 11       | 1.62          |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG12  | 11       | 1.62          |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG13  | 11       | 1.62          |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG11  | 11       | 1.62          |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG12  | 11       | 1.62          |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG13  | 11       | 1.62          |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG11  | 11       | 1.62          |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG12  | 11       | 1.62          |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG13  | 11       | 1.62          |
| (1,1645) | 1:77:A:ILE:HB   | 1:76:A:VAL:HG21  | 12       | 1.62          |
| (1,1645) | 1:77:A:ILE:HB   | 1:76:A:VAL:HG22  | 12       | 1.62          |
| (1,1645) | 1:77:A:ILE:HB   | 1:76:A:VAL:HG23  | 12       | 1.62          |
| (1,2561) | 1:6:A:PHE:HD1   | 1:123:A:VAL:HG11 | 7        | 1.61          |
| (1,2561) | 1:6:A:PHE:HD1   | 1:123:A:VAL:HG12 | 7        | 1.61          |
| (1,2561) | 1:6:A:PHE:HD1   | 1:123:A:VAL:HG13 | 7        | 1.61          |
| (1,2561) | 1:6:A:PHE:HD2   | 1:123:A:VAL:HG11 | 7        | 1.61          |
| (1,2561) | 1:6:A:PHE:HD2   | 1:123:A:VAL:HG12 | 7        | 1.61          |
| (1,2561) | 1:6:A:PHE:HD2   | 1:123:A:VAL:HG13 | 7        | 1.61          |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG11  | 9        | 1.61          |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG12  | 9        | 1.61          |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG13  | 9        | 1.61          |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG11  | 9        | 1.61          |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG12  | 9        | 1.61          |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG13  | 9        | 1.61          |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG11  | 9        | 1.61          |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG12  | 9        | 1.61          |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG13  | 9        | 1.61          |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG11  | 16       | 1.61          |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG12  | 16       | 1.61          |
| (1,1885) | 1:92:A:THR:HG21 | 1:91:A:VAL:HG13  | 16       | 1.61          |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG11  | 16       | 1.61          |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG12  | 16       | 1.61          |
| (1,1885) | 1:92:A:THR:HG22 | 1:91:A:VAL:HG13  | 16       | 1.61          |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG11  | 16       | 1.61          |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG12  | 16       | 1.61          |
| (1,1885) | 1:92:A:THR:HG23 | 1:91:A:VAL:HG13  | 16       | 1.61          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG21 | 18       | 1.61          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG22 | 18       | 1.61          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG23 | 18       | 1.61          |
| (1,814)  | 1:25:A:LEU:HB3  | 1:123:A:VAL:HG21 | 18       | 1.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 18       | 1.61          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 18       | 1.61          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 10       | 1.61          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 10       | 1.61          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 10       | 1.61          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 10       | 1.61          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 10       | 1.61          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 10       | 1.61          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 10       | 1.61          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 10       | 1.61          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 10       | 1.61          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 17       | 1.61          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 17       | 1.61          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 17       | 1.61          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11   | 17       | 1.61          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12   | 17       | 1.61          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13   | 17       | 1.61          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11   | 17       | 1.61          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12   | 17       | 1.61          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13   | 17       | 1.61          |
| (1,3711) | 1:79:A:LEU:HD11  | 1:16:A:GLN:H     | 15       | 1.6           |
| (1,3711) | 1:79:A:LEU:HD12  | 1:16:A:GLN:H     | 15       | 1.6           |
| (1,3711) | 1:79:A:LEU:HD13  | 1:16:A:GLN:H     | 15       | 1.6           |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 8        | 1.6           |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 8        | 1.6           |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 8        | 1.6           |
| (1,1885) | 1:92:A:THR:HG21  | 1:91:A:VAL:HG11  | 8        | 1.6           |
| (1,1885) | 1:92:A:THR:HG21  | 1:91:A:VAL:HG12  | 8        | 1.6           |
| (1,1885) | 1:92:A:THR:HG21  | 1:91:A:VAL:HG13  | 8        | 1.6           |
| (1,1885) | 1:92:A:THR:HG22  | 1:91:A:VAL:HG11  | 8        | 1.6           |
| (1,1885) | 1:92:A:THR:HG22  | 1:91:A:VAL:HG12  | 8        | 1.6           |
| (1,1885) | 1:92:A:THR:HG22  | 1:91:A:VAL:HG13  | 8        | 1.6           |
| (1,1885) | 1:92:A:THR:HG23  | 1:91:A:VAL:HG11  | 8        | 1.6           |
| (1,1885) | 1:92:A:THR:HG23  | 1:91:A:VAL:HG12  | 8        | 1.6           |
| (1,1885) | 1:92:A:THR:HG23  | 1:91:A:VAL:HG13  | 8        | 1.6           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 8        | 1.6           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 8        | 1.6           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 8        | 1.6           |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 2        | 1.6           |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 2        | 1.6           |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 2        | 1.6           |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 2        | 1.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 2        | 1.6           |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 2        | 1.6           |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 2        | 1.6           |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 2        | 1.6           |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 2        | 1.6           |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 12       | 1.6           |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 12       | 1.6           |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 12       | 1.6           |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 12       | 1.6           |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 12       | 1.6           |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 12       | 1.6           |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 12       | 1.6           |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 12       | 1.6           |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 12       | 1.6           |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 10       | 1.59          |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 10       | 1.59          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 10       | 1.59          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 8        | 1.59          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 8        | 1.59          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 8        | 1.59          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 8        | 1.59          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 8        | 1.59          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 8        | 1.59          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 8        | 1.59          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 8        | 1.59          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 8        | 1.59          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 8        | 1.59          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 8        | 1.59          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 8        | 1.59          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 14       | 1.59          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 14       | 1.59          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 14       | 1.59          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 14       | 1.59          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 14       | 1.59          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 14       | 1.59          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 8        | 1.59          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 8        | 1.59          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 8        | 1.59          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 8        | 1.59          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 8        | 1.59          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 8        | 1.59          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 10       | 1.59          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,808)  | 1:34:A:SER:H    | 1:32:A:VAL:HG12  | 10       | 1.59          |
| (1,808)  | 1:34:A:SER:H    | 1:32:A:VAL:HG13  | 10       | 1.59          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG21   | 13       | 1.59          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG22   | 13       | 1.59          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG23   | 13       | 1.59          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG21   | 13       | 1.59          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG22   | 13       | 1.59          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG23   | 13       | 1.59          |
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG21   | 13       | 1.59          |
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG22   | 13       | 1.59          |
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG23   | 13       | 1.59          |
| (1,3025) | 1:32:A:VAL:HG11 | 1:34:A:SER:H     | 20       | 1.58          |
| (1,3025) | 1:32:A:VAL:HG12 | 1:34:A:SER:H     | 20       | 1.58          |
| (1,3025) | 1:32:A:VAL:HG13 | 1:34:A:SER:H     | 20       | 1.58          |
| (1,1814) | 1:91:A:VAL:H    | 1:86:A:LEU:HD21  | 4        | 1.58          |
| (1,1814) | 1:91:A:VAL:H    | 1:86:A:LEU:HD22  | 4        | 1.58          |
| (1,1814) | 1:91:A:VAL:H    | 1:86:A:LEU:HD23  | 4        | 1.58          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG21 | 2        | 1.58          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG22 | 2        | 1.58          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG23 | 2        | 1.58          |
| (1,814)  | 1:25:A:LEU:HB3  | 1:123:A:VAL:HG21 | 2        | 1.58          |
| (1,814)  | 1:25:A:LEU:HB3  | 1:123:A:VAL:HG22 | 2        | 1.58          |
| (1,814)  | 1:25:A:LEU:HB3  | 1:123:A:VAL:HG23 | 2        | 1.58          |
| (1,808)  | 1:34:A:SER:H    | 1:32:A:VAL:HG11  | 20       | 1.58          |
| (1,808)  | 1:34:A:SER:H    | 1:32:A:VAL:HG12  | 20       | 1.58          |
| (1,808)  | 1:34:A:SER:H    | 1:32:A:VAL:HG13  | 20       | 1.58          |
| (1,3711) | 1:79:A:LEU:HD11 | 1:16:A:GLN:H     | 18       | 1.57          |
| (1,3711) | 1:79:A:LEU:HD12 | 1:16:A:GLN:H     | 18       | 1.57          |
| (1,3711) | 1:79:A:LEU:HD13 | 1:16:A:GLN:H     | 18       | 1.57          |
| (1,3025) | 1:32:A:VAL:HG11 | 1:34:A:SER:H     | 6        | 1.57          |
| (1,3025) | 1:32:A:VAL:HG12 | 1:34:A:SER:H     | 6        | 1.57          |
| (1,3025) | 1:32:A:VAL:HG13 | 1:34:A:SER:H     | 6        | 1.57          |
| (1,808)  | 1:34:A:SER:H    | 1:32:A:VAL:HG11  | 6        | 1.57          |
| (1,808)  | 1:34:A:SER:H    | 1:32:A:VAL:HG12  | 6        | 1.57          |
| (1,808)  | 1:34:A:SER:H    | 1:32:A:VAL:HG13  | 6        | 1.57          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG21   | 4        | 1.57          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG22   | 4        | 1.57          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG23   | 4        | 1.57          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG21   | 4        | 1.57          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG22   | 4        | 1.57          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG23   | 4        | 1.57          |
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG21   | 4        | 1.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 4        | 1.57          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 4        | 1.57          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 6        | 1.56          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 6        | 1.56          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 6        | 1.56          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 6        | 1.56          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 6        | 1.56          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 6        | 1.56          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 6        | 1.56          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 6        | 1.56          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 6        | 1.56          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 17       | 1.56          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 17       | 1.56          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 17       | 1.56          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 6        | 1.56          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 6        | 1.56          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 6        | 1.56          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 6        | 1.56          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 6        | 1.56          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 6        | 1.56          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 3        | 1.56          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 3        | 1.56          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 3        | 1.56          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 3        | 1.56          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 3        | 1.56          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 3        | 1.56          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 3        | 1.56          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 3        | 1.56          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 3        | 1.56          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 3        | 1.55          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 3        | 1.55          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 3        | 1.55          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 3        | 1.55          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 3        | 1.55          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 3        | 1.55          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 14       | 1.55          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 14       | 1.55          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 14       | 1.55          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 14       | 1.55          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 14       | 1.55          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 14       | 1.55          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 15       | 1.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 15       | 1.54          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 15       | 1.54          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 15       | 1.54          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 15       | 1.54          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 15       | 1.54          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 20       | 1.54          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 20       | 1.54          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 20       | 1.54          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 13       | 1.53          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 13       | 1.53          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 13       | 1.53          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 13       | 1.53          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 13       | 1.53          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 13       | 1.53          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 13       | 1.53          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 13       | 1.53          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 13       | 1.53          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 13       | 1.53          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 13       | 1.53          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 13       | 1.53          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 17       | 1.53          |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 17       | 1.53          |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 17       | 1.53          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 17       | 1.53          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 17       | 1.53          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 17       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 15       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 15       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 15       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 15       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 15       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 15       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 15       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 15       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 15       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 18       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 18       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 18       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 18       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 18       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 18       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 18       | 1.53          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG22   | 18       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG23   | 18       | 1.53          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG21   | 14       | 1.52          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG22   | 14       | 1.52          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG23   | 14       | 1.52          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG21   | 14       | 1.52          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG22   | 14       | 1.52          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG23   | 14       | 1.52          |
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG21   | 14       | 1.52          |
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG22   | 14       | 1.52          |
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG23   | 14       | 1.52          |
| (1,2561) | 1:6:A:PHE:HD1   | 1:123:A:VAL:HG11 | 10       | 1.51          |
| (1,2561) | 1:6:A:PHE:HD1   | 1:123:A:VAL:HG12 | 10       | 1.51          |
| (1,2561) | 1:6:A:PHE:HD1   | 1:123:A:VAL:HG13 | 10       | 1.51          |
| (1,2561) | 1:6:A:PHE:HD2   | 1:123:A:VAL:HG11 | 10       | 1.51          |
| (1,2561) | 1:6:A:PHE:HD2   | 1:123:A:VAL:HG12 | 10       | 1.51          |
| (1,2561) | 1:6:A:PHE:HD2   | 1:123:A:VAL:HG13 | 10       | 1.51          |
| (1,1645) | 1:77:A:ILE:HB   | 1:76:A:VAL:HG21  | 4        | 1.51          |
| (1,1645) | 1:77:A:ILE:HB   | 1:76:A:VAL:HG22  | 4        | 1.51          |
| (1,1645) | 1:77:A:ILE:HB   | 1:76:A:VAL:HG23  | 4        | 1.51          |
| (1,1645) | 1:77:A:ILE:HB   | 1:76:A:VAL:HG21  | 13       | 1.51          |
| (1,1645) | 1:77:A:ILE:HB   | 1:76:A:VAL:HG22  | 13       | 1.51          |
| (1,1645) | 1:77:A:ILE:HB   | 1:76:A:VAL:HG23  | 13       | 1.51          |
| (1,1240) | 1:116:A:ARG:HG2 | 1:53:A:VAL:HG11  | 3        | 1.51          |
| (1,1240) | 1:116:A:ARG:HG2 | 1:53:A:VAL:HG12  | 3        | 1.51          |
| (1,1240) | 1:116:A:ARG:HG2 | 1:53:A:VAL:HG13  | 3        | 1.51          |
| (1,1240) | 1:116:A:ARG:HG3 | 1:53:A:VAL:HG11  | 3        | 1.51          |
| (1,1240) | 1:116:A:ARG:HG3 | 1:53:A:VAL:HG12  | 3        | 1.51          |
| (1,1240) | 1:116:A:ARG:HG3 | 1:53:A:VAL:HG13  | 3        | 1.51          |
| (1,822)  | 1:31:A:ALA:H    | 1:32:A:VAL:HG21  | 17       | 1.51          |
| (1,822)  | 1:31:A:ALA:H    | 1:32:A:VAL:HG22  | 17       | 1.51          |
| (1,822)  | 1:31:A:ALA:H    | 1:32:A:VAL:HG23  | 17       | 1.51          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG21   | 1        | 1.51          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG22   | 1        | 1.51          |
| (1,278)  | 1:32:A:VAL:HG21 | 1:4:A:VAL:HG23   | 1        | 1.51          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG21   | 1        | 1.51          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG22   | 1        | 1.51          |
| (1,278)  | 1:32:A:VAL:HG22 | 1:4:A:VAL:HG23   | 1        | 1.51          |
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG21   | 1        | 1.51          |
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG22   | 1        | 1.51          |
| (1,278)  | 1:32:A:VAL:HG23 | 1:4:A:VAL:HG23   | 1        | 1.51          |
| (1,3025) | 1:32:A:VAL:HG11 | 1:34:A:SER:H     | 2        | 1.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 2        | 1.49          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 2        | 1.49          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 11       | 1.49          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 11       | 1.49          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 11       | 1.49          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 11       | 1.49          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 11       | 1.49          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 11       | 1.49          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 8        | 1.49          |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 8        | 1.49          |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 8        | 1.49          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 2        | 1.49          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 2        | 1.49          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 2        | 1.49          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 19       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 19       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 19       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 19       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 19       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 19       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 19       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 19       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 19       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 20       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 20       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 20       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 20       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 20       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 20       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 20       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 20       | 1.49          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 20       | 1.49          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 4        | 1.48          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 4        | 1.48          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 4        | 1.48          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 4        | 1.48          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 4        | 1.48          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 4        | 1.48          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 4        | 1.48          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 4        | 1.48          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 4        | 1.48          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 4        | 1.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 4        | 1.48          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 4        | 1.48          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 5        | 1.48          |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 5        | 1.48          |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 5        | 1.48          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 6        | 1.48          |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 6        | 1.48          |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 6        | 1.48          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 5        | 1.48          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 5        | 1.48          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 5        | 1.48          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 5        | 1.48          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 5        | 1.48          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 5        | 1.48          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 5        | 1.48          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 5        | 1.48          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 5        | 1.48          |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 13       | 1.47          |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 13       | 1.47          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 13       | 1.47          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 1        | 1.47          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 1        | 1.47          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 1        | 1.47          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 1        | 1.47          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 1        | 1.47          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 1        | 1.47          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 9        | 1.47          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 9        | 1.47          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 9        | 1.47          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 9        | 1.47          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 9        | 1.47          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 9        | 1.47          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 9        | 1.47          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 9        | 1.47          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 9        | 1.47          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 19       | 1.47          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 19       | 1.47          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 19       | 1.47          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 13       | 1.47          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 13       | 1.47          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 13       | 1.47          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2   | 4        | 1.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3   | 4        | 1.47          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2   | 4        | 1.47          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3   | 4        | 1.47          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2   | 4        | 1.47          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3   | 4        | 1.47          |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 19       | 1.46          |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 19       | 1.46          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 19       | 1.46          |
| (1,2769) | 1:4:A:VAL:HG21   | 1:30:A:ILE:HB    | 13       | 1.46          |
| (1,2769) | 1:4:A:VAL:HG22   | 1:30:A:ILE:HB    | 13       | 1.46          |
| (1,2769) | 1:4:A:VAL:HG23   | 1:30:A:ILE:HB    | 13       | 1.46          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 2        | 1.46          |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 2        | 1.46          |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 2        | 1.46          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 7        | 1.46          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 7        | 1.46          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 7        | 1.46          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 19       | 1.46          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 19       | 1.46          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 19       | 1.46          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 1        | 1.45          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 1        | 1.45          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 1        | 1.45          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG21  | 5        | 1.45          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG22  | 5        | 1.45          |
| (1,1645) | 1:77:A:ILE:HB    | 1:76:A:VAL:HG23  | 5        | 1.45          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 12       | 1.45          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 12       | 1.45          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 12       | 1.45          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 12       | 1.45          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 12       | 1.45          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 12       | 1.45          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 17       | 1.45          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 17       | 1.45          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 17       | 1.45          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 17       | 1.45          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 17       | 1.45          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 17       | 1.45          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 11       | 1.44          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 11       | 1.44          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 11       | 1.44          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 11       | 1.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 11       | 1.44          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 11       | 1.44          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 11       | 1.44          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 11       | 1.44          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 11       | 1.44          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG21  | 18       | 1.44          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG22  | 18       | 1.44          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG23  | 18       | 1.44          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG21  | 18       | 1.44          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG22  | 18       | 1.44          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG23  | 18       | 1.44          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG21  | 18       | 1.44          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG22  | 18       | 1.44          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG23  | 18       | 1.44          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 11       | 1.44          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 11       | 1.44          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 11       | 1.44          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 11       | 1.44          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 11       | 1.44          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 11       | 1.44          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 11       | 1.44          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 11       | 1.44          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 11       | 1.44          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11  | 15       | 1.43          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12  | 15       | 1.43          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13  | 15       | 1.43          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 2        | 1.43          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 2        | 1.43          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 2        | 1.43          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 3        | 1.43          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 3        | 1.43          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 3        | 1.43          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 20       | 1.43          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 20       | 1.43          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 20       | 1.43          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 20       | 1.43          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 20       | 1.43          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 20       | 1.43          |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 15       | 1.42          |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 15       | 1.42          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 15       | 1.42          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 20       | 1.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 20       | 1.42          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 20       | 1.42          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 20       | 1.42          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 20       | 1.42          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 20       | 1.42          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 3        | 1.42          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 3        | 1.42          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 3        | 1.42          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 15       | 1.42          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 15       | 1.42          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 15       | 1.42          |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 14       | 1.41          |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 14       | 1.41          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 14       | 1.41          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 1        | 1.41          |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 1        | 1.41          |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 1        | 1.41          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 13       | 1.41          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 13       | 1.41          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 13       | 1.41          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 13       | 1.41          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 13       | 1.41          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 13       | 1.41          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 8        | 1.41          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 8        | 1.41          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 8        | 1.41          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 20       | 1.41          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 20       | 1.41          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 20       | 1.41          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 14       | 1.41          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 14       | 1.41          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 14       | 1.41          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 8        | 1.41          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 8        | 1.41          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 8        | 1.41          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 8        | 1.41          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 8        | 1.41          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 8        | 1.41          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 8        | 1.41          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 8        | 1.41          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 8        | 1.41          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG11   | 13       | 1.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG12   | 13       | 1.41          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG13   | 13       | 1.41          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 4        | 1.4           |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 4        | 1.4           |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 4        | 1.4           |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 12       | 1.4           |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 12       | 1.4           |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 12       | 1.4           |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 1        | 1.39          |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 1        | 1.39          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 1        | 1.39          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 15       | 1.39          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 15       | 1.39          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 15       | 1.39          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 7        | 1.39          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 7        | 1.39          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 7        | 1.39          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 7        | 1.39          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 7        | 1.39          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 7        | 1.39          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 15       | 1.39          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 15       | 1.39          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 15       | 1.39          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 18       | 1.39          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 18       | 1.39          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 18       | 1.39          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 19       | 1.39          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 19       | 1.39          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 19       | 1.39          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 1        | 1.39          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 1        | 1.39          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 1        | 1.39          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG21  | 5        | 1.38          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG22  | 5        | 1.38          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG23  | 5        | 1.38          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG21  | 5        | 1.38          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG22  | 5        | 1.38          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG23  | 5        | 1.38          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG21  | 5        | 1.38          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG22  | 5        | 1.38          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG23  | 5        | 1.38          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD11  | 9        | 1.38          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD12 | 9        | 1.38          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD13 | 9        | 1.38          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD11 | 9        | 1.38          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD12 | 9        | 1.38          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD13 | 9        | 1.38          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD11 | 9        | 1.38          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD12 | 9        | 1.38          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD13 | 9        | 1.38          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21 | 14       | 1.38          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22 | 14       | 1.38          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23 | 14       | 1.38          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2  | 16       | 1.38          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3  | 16       | 1.38          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2  | 16       | 1.38          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3  | 16       | 1.38          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2  | 16       | 1.38          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3  | 16       | 1.38          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA  | 20       | 1.37          |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA  | 20       | 1.37          |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA  | 20       | 1.37          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 3        | 1.37          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 3        | 1.37          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 3        | 1.37          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 3        | 1.37          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 3        | 1.37          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 3        | 1.37          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 3        | 1.37          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 3        | 1.37          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 3        | 1.37          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 3        | 1.37          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 3        | 1.37          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 3        | 1.37          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11 | 10       | 1.37          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12 | 10       | 1.37          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13 | 10       | 1.37          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11 | 10       | 1.37          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12 | 10       | 1.37          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13 | 10       | 1.37          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11 | 4        | 1.37          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12 | 4        | 1.37          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13 | 4        | 1.37          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21 | 7        | 1.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 7        | 1.37          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 7        | 1.37          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 2        | 1.37          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 2        | 1.37          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 2        | 1.37          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 2        | 1.37          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 2        | 1.37          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 2        | 1.37          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 2        | 1.37          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 2        | 1.37          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 2        | 1.37          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 2        | 1.37          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 2        | 1.37          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 2        | 1.37          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 14       | 1.36          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 14       | 1.36          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 14       | 1.36          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 14       | 1.36          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 14       | 1.36          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 14       | 1.36          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 14       | 1.36          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 14       | 1.36          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 14       | 1.36          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 14       | 1.36          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 14       | 1.36          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 14       | 1.36          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 3        | 1.36          |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 3        | 1.36          |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 3        | 1.36          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 19       | 1.36          |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 19       | 1.36          |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 19       | 1.36          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 8        | 1.36          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 8        | 1.36          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 8        | 1.36          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 8        | 1.36          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 8        | 1.36          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 8        | 1.36          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 8        | 1.36          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 8        | 1.36          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 8        | 1.36          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11  | 7        | 1.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12  | 7        | 1.36          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13  | 7        | 1.36          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11  | 7        | 1.36          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12  | 7        | 1.36          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13  | 7        | 1.36          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 10       | 1.36          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 10       | 1.36          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 10       | 1.36          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 12       | 1.36          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 12       | 1.36          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 12       | 1.36          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 1        | 1.36          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 1        | 1.36          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 1        | 1.36          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 1        | 1.36          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 1        | 1.36          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 1        | 1.36          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 18       | 1.35          |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 18       | 1.35          |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 18       | 1.35          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 3        | 1.35          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 3        | 1.35          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 3        | 1.35          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 3        | 1.35          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 3        | 1.35          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 3        | 1.35          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 3        | 1.35          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 3        | 1.35          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 3        | 1.35          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 5        | 1.35          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 5        | 1.35          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 5        | 1.35          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 5        | 1.35          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 5        | 1.35          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 5        | 1.35          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2   | 10       | 1.35          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3   | 10       | 1.35          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2   | 10       | 1.35          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3   | 10       | 1.35          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2   | 10       | 1.35          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3   | 10       | 1.35          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 9        | 1.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 9        | 1.35          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 9        | 1.35          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 9        | 1.35          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 9        | 1.35          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 9        | 1.35          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 9        | 1.35          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 9        | 1.35          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 9        | 1.35          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 9        | 1.35          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 9        | 1.35          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 9        | 1.35          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21   | 11       | 1.35          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22   | 11       | 1.35          |
| (1,278)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23   | 11       | 1.35          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21   | 11       | 1.35          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22   | 11       | 1.35          |
| (1,278)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23   | 11       | 1.35          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21   | 11       | 1.35          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22   | 11       | 1.35          |
| (1,278)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23   | 11       | 1.35          |
| (1,268)  | 1:75:A:VAL:HA    | 1:4:A:VAL:HG21   | 6        | 1.35          |
| (1,268)  | 1:75:A:VAL:HA    | 1:4:A:VAL:HG22   | 6        | 1.35          |
| (1,268)  | 1:75:A:VAL:HA    | 1:4:A:VAL:HG23   | 6        | 1.35          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG11   | 7        | 1.35          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG12   | 7        | 1.35          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG13   | 7        | 1.35          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 20       | 1.34          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 20       | 1.34          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 20       | 1.34          |
| (1,2398) | 1:123:A:VAL:HG11 | 1:119:A:VAL:HA   | 14       | 1.34          |
| (1,2398) | 1:123:A:VAL:HG12 | 1:119:A:VAL:HA   | 14       | 1.34          |
| (1,2398) | 1:123:A:VAL:HG13 | 1:119:A:VAL:HA   | 14       | 1.34          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 15       | 1.34          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 15       | 1.34          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 15       | 1.34          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 6        | 1.34          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 6        | 1.34          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 6        | 1.34          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 20       | 1.32          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 20       | 1.32          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 20       | 1.32          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 20       | 1.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 20       | 1.32          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 20       | 1.32          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 20       | 1.32          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 20       | 1.32          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 20       | 1.32          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 16       | 1.32          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 16       | 1.32          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 16       | 1.32          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 16       | 1.32          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 16       | 1.32          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 16       | 1.32          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11  | 19       | 1.32          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12  | 19       | 1.32          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13  | 19       | 1.32          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG21  | 4        | 1.32          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG22  | 4        | 1.32          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG23  | 4        | 1.32          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG21  | 4        | 1.32          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG22  | 4        | 1.32          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG23  | 4        | 1.32          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG21  | 4        | 1.32          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG22  | 4        | 1.32          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG23  | 4        | 1.32          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 15       | 1.32          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 15       | 1.32          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 15       | 1.32          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG11  | 11       | 1.31          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG12  | 11       | 1.31          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG13  | 11       | 1.31          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG11  | 11       | 1.31          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG12  | 11       | 1.31          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG13  | 11       | 1.31          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1   | 16       | 1.3           |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1   | 16       | 1.3           |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1   | 16       | 1.3           |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 11       | 1.3           |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 11       | 1.3           |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 11       | 1.3           |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 16       | 1.3           |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 16       | 1.3           |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 16       | 1.3           |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 18       | 1.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 18       | 1.3           |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 18       | 1.3           |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 15       | 1.3           |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 15       | 1.3           |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 15       | 1.3           |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 15       | 1.3           |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 15       | 1.3           |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 15       | 1.3           |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 15       | 1.3           |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 15       | 1.3           |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 15       | 1.3           |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 15       | 1.3           |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 15       | 1.3           |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 15       | 1.3           |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 11       | 1.3           |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 11       | 1.3           |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 11       | 1.3           |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 11       | 1.3           |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 11       | 1.3           |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 11       | 1.3           |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 11       | 1.3           |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 11       | 1.3           |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 11       | 1.3           |
| (1,883)  | 1:86:A:LEU:HD21  | 1:37:A:LEU:HA    | 17       | 1.3           |
| (1,883)  | 1:86:A:LEU:HD22  | 1:37:A:LEU:HA    | 17       | 1.3           |
| (1,883)  | 1:86:A:LEU:HD23  | 1:37:A:LEU:HA    | 17       | 1.3           |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 16       | 1.3           |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 16       | 1.3           |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 16       | 1.3           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 11       | 1.3           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 11       | 1.3           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 11       | 1.3           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 16       | 1.3           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 16       | 1.3           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 16       | 1.3           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 18       | 1.3           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 18       | 1.3           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 18       | 1.3           |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 19       | 1.29          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 19       | 1.29          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 19       | 1.29          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 19       | 1.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 19       | 1.29          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 19       | 1.29          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 19       | 1.29          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 19       | 1.29          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 19       | 1.29          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 19       | 1.29          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 19       | 1.29          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 19       | 1.29          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 4        | 1.29          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 4        | 1.29          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 4        | 1.29          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 4        | 1.29          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 4        | 1.29          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 4        | 1.29          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 1        | 1.29          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 1        | 1.29          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 1        | 1.29          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 9        | 1.28          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 9        | 1.28          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 9        | 1.28          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 9        | 1.28          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 9        | 1.28          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 9        | 1.28          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 14       | 1.28          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 14       | 1.28          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 14       | 1.28          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 2        | 1.28          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 2        | 1.28          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 2        | 1.28          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 10       | 1.28          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 10       | 1.28          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 10       | 1.28          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 10       | 1.28          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 10       | 1.28          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 10       | 1.28          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 10       | 1.28          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 10       | 1.28          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 10       | 1.28          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 10       | 1.28          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 10       | 1.28          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 10       | 1.28          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 10       | 1.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 10       | 1.28          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 10       | 1.28          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 10       | 1.28          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 10       | 1.28          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 10       | 1.28          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 10       | 1.28          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 10       | 1.28          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 10       | 1.28          |
| (1,244)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HB     | 7        | 1.28          |
| (1,244)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HB     | 7        | 1.28          |
| (1,244)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HB     | 7        | 1.28          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 4        | 1.27          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 4        | 1.27          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 4        | 1.27          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 16       | 1.27          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 16       | 1.27          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 16       | 1.27          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 18       | 1.27          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 18       | 1.27          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 18       | 1.27          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 18       | 1.27          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 18       | 1.27          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 18       | 1.27          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 13       | 1.27          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 13       | 1.27          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 13       | 1.27          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 13       | 1.27          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 13       | 1.27          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 13       | 1.27          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 13       | 1.27          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 13       | 1.27          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 13       | 1.27          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 17       | 1.27          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 17       | 1.27          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 17       | 1.27          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 17       | 1.27          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 17       | 1.27          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 17       | 1.27          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 17       | 1.27          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 17       | 1.27          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 17       | 1.27          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 17       | 1.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 17       | 1.27          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 17       | 1.27          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 9        | 1.26          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 9        | 1.26          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 9        | 1.26          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 9        | 1.26          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 9        | 1.26          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 9        | 1.26          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 1        | 1.26          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 1        | 1.26          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 1        | 1.26          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 1        | 1.26          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 1        | 1.26          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 1        | 1.26          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 9        | 1.26          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 9        | 1.26          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 9        | 1.26          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 9        | 1.26          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 9        | 1.26          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 9        | 1.26          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 17       | 1.26          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 17       | 1.26          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 17       | 1.26          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 17       | 1.26          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 17       | 1.26          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 17       | 1.26          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 1        | 1.26          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 1        | 1.26          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 1        | 1.26          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 1        | 1.26          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 1        | 1.26          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 1        | 1.26          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 1        | 1.26          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 1        | 1.26          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 1        | 1.26          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 1        | 1.26          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 1        | 1.26          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 1        | 1.26          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 6        | 1.26          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 6        | 1.26          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 6        | 1.26          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 6        | 1.26          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22 | 6        | 1.26          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23 | 6        | 1.26          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21 | 6        | 1.26          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22 | 6        | 1.26          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23 | 6        | 1.26          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11 | 1        | 1.26          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12 | 1        | 1.26          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13 | 1        | 1.26          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21 | 9        | 1.26          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22 | 9        | 1.26          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23 | 9        | 1.26          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2   | 16       | 1.26          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3   | 16       | 1.26          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2   | 16       | 1.26          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3   | 16       | 1.26          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2   | 16       | 1.26          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3   | 16       | 1.26          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2   | 19       | 1.26          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3   | 19       | 1.26          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2   | 19       | 1.26          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3   | 19       | 1.26          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2   | 19       | 1.26          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3   | 19       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2   | 16       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3   | 16       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2   | 16       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3   | 16       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2   | 16       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3   | 16       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2   | 19       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3   | 19       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2   | 19       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3   | 19       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2   | 19       | 1.26          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3   | 19       | 1.26          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H    | 14       | 1.25          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H    | 14       | 1.25          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H    | 14       | 1.25          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11 | 2        | 1.25          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12 | 2        | 1.25          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13 | 2        | 1.25          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG21 | 14       | 1.25          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 14       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 14       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 14       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 14       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 14       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 14       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 14       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 14       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG21  | 16       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 16       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 16       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 16       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 16       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 16       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 16       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 16       | 1.25          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 16       | 1.25          |
| (1,822)  | 1:31:A:ALA:H    | 1:32:A:VAL:HG21  | 18       | 1.25          |
| (1,822)  | 1:31:A:ALA:H    | 1:32:A:VAL:HG22  | 18       | 1.25          |
| (1,822)  | 1:31:A:ALA:H    | 1:32:A:VAL:HG23  | 18       | 1.25          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD11 | 13       | 1.25          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD12 | 13       | 1.25          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD13 | 13       | 1.25          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD11 | 13       | 1.25          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD12 | 13       | 1.25          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD13 | 13       | 1.25          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD11 | 13       | 1.25          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD12 | 13       | 1.25          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD13 | 13       | 1.25          |
| (1,259)  | 1:75:A:VAL:HB   | 1:4:A:VAL:HG11   | 17       | 1.25          |
| (1,259)  | 1:75:A:VAL:HB   | 1:4:A:VAL:HG12   | 17       | 1.25          |
| (1,259)  | 1:75:A:VAL:HB   | 1:4:A:VAL:HG13   | 17       | 1.25          |
| (1,49)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG2   | 5        | 1.25          |
| (1,49)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG3   | 5        | 1.25          |
| (1,49)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG2   | 5        | 1.25          |
| (1,49)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG3   | 5        | 1.25          |
| (1,49)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG2   | 5        | 1.25          |
| (1,49)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG3   | 5        | 1.25          |
| (1,47)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG2   | 5        | 1.25          |
| (1,47)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG3   | 5        | 1.25          |
| (1,47)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG2   | 5        | 1.25          |
| (1,47)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG3   | 5        | 1.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 5        | 1.25          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 5        | 1.25          |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H     | 4        | 1.24          |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H     | 4        | 1.24          |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H     | 4        | 1.24          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 19       | 1.24          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 19       | 1.24          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 19       | 1.24          |
| (1,2769) | 1:4:A:VAL:HG21   | 1:30:A:ILE:HB    | 17       | 1.24          |
| (1,2769) | 1:4:A:VAL:HG22   | 1:30:A:ILE:HB    | 17       | 1.24          |
| (1,2769) | 1:4:A:VAL:HG23   | 1:30:A:ILE:HB    | 17       | 1.24          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 8        | 1.24          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 8        | 1.24          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 8        | 1.24          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 8        | 1.24          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 8        | 1.24          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 8        | 1.24          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 8        | 1.24          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 8        | 1.24          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 8        | 1.24          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 8        | 1.24          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 8        | 1.24          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 8        | 1.24          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 5        | 1.24          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 5        | 1.24          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 5        | 1.24          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 4        | 1.24          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 4        | 1.24          |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 4        | 1.24          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11  | 13       | 1.24          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12  | 13       | 1.24          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13  | 13       | 1.24          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 13       | 1.24          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 13       | 1.24          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 13       | 1.24          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 17       | 1.23          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 17       | 1.23          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 17       | 1.23          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 17       | 1.23          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 17       | 1.23          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 17       | 1.23          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 17       | 1.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 17       | 1.23          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 17       | 1.23          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 17       | 1.23          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 17       | 1.23          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 17       | 1.23          |
| (1,2084) | 1:79:A:LEU:HD21  | 1:101:A:LEU:HG   | 10       | 1.23          |
| (1,2084) | 1:79:A:LEU:HD22  | 1:101:A:LEU:HG   | 10       | 1.23          |
| (1,2084) | 1:79:A:LEU:HD23  | 1:101:A:LEU:HG   | 10       | 1.23          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 15       | 1.23          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 15       | 1.23          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 15       | 1.23          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 15       | 1.23          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 15       | 1.23          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 15       | 1.23          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 15       | 1.23          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 15       | 1.23          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 15       | 1.23          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 6        | 1.23          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 6        | 1.23          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 6        | 1.23          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 6        | 1.23          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 6        | 1.23          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 6        | 1.23          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 11       | 1.23          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 11       | 1.23          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 11       | 1.23          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 11       | 1.23          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 11       | 1.23          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 11       | 1.23          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 6        | 1.23          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 6        | 1.23          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 6        | 1.23          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 6        | 1.23          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 6        | 1.23          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 6        | 1.23          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 11       | 1.23          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 11       | 1.23          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 11       | 1.23          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 11       | 1.23          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 11       | 1.23          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 11       | 1.23          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 7        | 1.22          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG22 | 7        | 1.22          |
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG23 | 7        | 1.22          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG21 | 7        | 1.22          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG22 | 7        | 1.22          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG23 | 7        | 1.22          |
| (1,911)  | 1:65:A:ILE:HB   | 1:37:A:LEU:HD11  | 8        | 1.22          |
| (1,911)  | 1:65:A:ILE:HB   | 1:37:A:LEU:HD12  | 8        | 1.22          |
| (1,911)  | 1:65:A:ILE:HB   | 1:37:A:LEU:HD13  | 8        | 1.22          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD11 | 6        | 1.22          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD12 | 6        | 1.22          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD13 | 6        | 1.22          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD11 | 6        | 1.22          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD12 | 6        | 1.22          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD13 | 6        | 1.22          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD11 | 6        | 1.22          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD12 | 6        | 1.22          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD13 | 6        | 1.22          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD11 | 14       | 1.22          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD12 | 14       | 1.22          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD13 | 14       | 1.22          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD11 | 14       | 1.22          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD12 | 14       | 1.22          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD13 | 14       | 1.22          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD11 | 14       | 1.22          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD12 | 14       | 1.22          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD13 | 14       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG2    | 13       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG3    | 13       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG2    | 13       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG3    | 13       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD23 | 1:9:A:LYS:HG2    | 13       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD23 | 1:9:A:LYS:HG3    | 13       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG2    | 20       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG3    | 20       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG2    | 20       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG3    | 20       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD23 | 1:9:A:LYS:HG2    | 20       | 1.22          |
| (1,370)  | 1:37:A:LEU:HD23 | 1:9:A:LYS:HG3    | 20       | 1.22          |
| (1,367)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG2    | 13       | 1.22          |
| (1,367)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG3    | 13       | 1.22          |
| (1,367)  | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG2    | 13       | 1.22          |
| (1,367)  | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG3    | 13       | 1.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2   | 13       | 1.22          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3   | 13       | 1.22          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2   | 20       | 1.22          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3   | 20       | 1.22          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2   | 20       | 1.22          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3   | 20       | 1.22          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2   | 20       | 1.22          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3   | 20       | 1.22          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H    | 10       | 1.21          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H    | 10       | 1.21          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H    | 10       | 1.21          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 5        | 1.21          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 5        | 1.21          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 5        | 1.21          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 5        | 1.21          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 5        | 1.21          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 5        | 1.21          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 19       | 1.21          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 19       | 1.21          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 19       | 1.21          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 19       | 1.21          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 19       | 1.21          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 19       | 1.21          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 5        | 1.21          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 5        | 1.21          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 5        | 1.21          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 5        | 1.21          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 5        | 1.21          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 5        | 1.21          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 19       | 1.21          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 19       | 1.21          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 19       | 1.21          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 19       | 1.21          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 19       | 1.21          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 19       | 1.21          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG21 | 11       | 1.21          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG22 | 11       | 1.21          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG23 | 11       | 1.21          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG21 | 11       | 1.21          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG22 | 11       | 1.21          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG23 | 11       | 1.21          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG21 | 11       | 1.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG22  | 11       | 1.21          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG23  | 11       | 1.21          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11  | 17       | 1.21          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12  | 17       | 1.21          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13  | 17       | 1.21          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11  | 17       | 1.21          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12  | 17       | 1.21          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13  | 17       | 1.21          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 20       | 1.21          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 20       | 1.21          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 20       | 1.21          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG21  | 4        | 1.21          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG22  | 4        | 1.21          |
| (1,822)  | 1:31:A:ALA:H     | 1:32:A:VAL:HG23  | 4        | 1.21          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 2        | 1.21          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 2        | 1.21          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 2        | 1.21          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 2        | 1.21          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 2        | 1.21          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 2        | 1.21          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 2        | 1.21          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 2        | 1.21          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 2        | 1.21          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 2        | 1.21          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 2        | 1.21          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 2        | 1.21          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 1        | 1.2           |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 1        | 1.2           |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 1        | 1.2           |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 19       | 1.2           |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 19       | 1.2           |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 19       | 1.2           |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 19       | 1.2           |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 19       | 1.2           |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 19       | 1.2           |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 19       | 1.2           |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 19       | 1.2           |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 19       | 1.2           |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 13       | 1.2           |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 13       | 1.2           |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 13       | 1.2           |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 10       | 1.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 10       | 1.2           |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 10       | 1.2           |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 10       | 1.2           |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 10       | 1.2           |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 10       | 1.2           |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 20       | 1.2           |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 20       | 1.2           |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 20       | 1.2           |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 20       | 1.2           |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 20       | 1.2           |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 20       | 1.2           |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 20       | 1.2           |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 20       | 1.2           |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 20       | 1.2           |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 20       | 1.2           |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 20       | 1.2           |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 20       | 1.2           |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 13       | 1.2           |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 13       | 1.2           |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 13       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 14       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 14       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 14       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 14       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 14       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 14       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 18       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 18       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 18       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 18       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 18       | 1.2           |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 18       | 1.2           |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 14       | 1.2           |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 14       | 1.2           |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 14       | 1.2           |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 14       | 1.2           |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 14       | 1.2           |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 14       | 1.2           |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 18       | 1.2           |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 18       | 1.2           |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 18       | 1.2           |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 18       | 1.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 18       | 1.2           |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 18       | 1.2           |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 3        | 1.19          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 3        | 1.19          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 3        | 1.19          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 3        | 1.19          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 3        | 1.19          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 3        | 1.19          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 3        | 1.19          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 3        | 1.19          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 3        | 1.19          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 3        | 1.19          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 3        | 1.19          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 3        | 1.19          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG11  | 4        | 1.19          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG12  | 4        | 1.19          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG13  | 4        | 1.19          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG11  | 4        | 1.19          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG12  | 4        | 1.19          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG13  | 4        | 1.19          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2   | 1        | 1.19          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3   | 1        | 1.19          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2   | 1        | 1.19          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3   | 1        | 1.19          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2   | 1        | 1.19          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3   | 1        | 1.19          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 4        | 1.19          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 4        | 1.19          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 4        | 1.19          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 4        | 1.19          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 4        | 1.19          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 4        | 1.19          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 15       | 1.19          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 15       | 1.19          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 15       | 1.19          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 15       | 1.19          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 15       | 1.19          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 15       | 1.19          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 4        | 1.19          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 4        | 1.19          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 4        | 1.19          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 4        | 1.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 4        | 1.19          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 4        | 1.19          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 15       | 1.19          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 15       | 1.19          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 15       | 1.19          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 15       | 1.19          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 15       | 1.19          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 15       | 1.19          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 11       | 1.18          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 11       | 1.18          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 11       | 1.18          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 11       | 1.18          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 11       | 1.18          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 11       | 1.18          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 15       | 1.18          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 15       | 1.18          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 15       | 1.18          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 15       | 1.18          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 15       | 1.18          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 15       | 1.18          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 15       | 1.18          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 15       | 1.18          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 15       | 1.18          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG21  | 15       | 1.18          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG22  | 15       | 1.18          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG23  | 15       | 1.18          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG21  | 15       | 1.18          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG22  | 15       | 1.18          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG23  | 15       | 1.18          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG21  | 15       | 1.18          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG22  | 15       | 1.18          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG23  | 15       | 1.18          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 5        | 1.18          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 5        | 1.18          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 5        | 1.18          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 5        | 1.18          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 5        | 1.18          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 5        | 1.18          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 5        | 1.18          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 5        | 1.18          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 5        | 1.18          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 5        | 1.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 5        | 1.18          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 5        | 1.18          |
| (1,244)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HB     | 17       | 1.18          |
| (1,244)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HB     | 17       | 1.18          |
| (1,244)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HB     | 17       | 1.18          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 1        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 1        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 1        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 1        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 1        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 1        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 1        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 1        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 1        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 2        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 2        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 2        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 2        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 2        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 2        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 2        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 2        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 2        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 4        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 4        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 4        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 4        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 4        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 4        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 4        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 4        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 4        | 1.17          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 16       | 1.17          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 16       | 1.17          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 16       | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 16       | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 16       | 1.17          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 16       | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 16       | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 16       | 1.17          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 16       | 1.17          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 15       | 1.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD22 | 15       | 1.17          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD23 | 15       | 1.17          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD21 | 15       | 1.17          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD22 | 15       | 1.17          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD23 | 15       | 1.17          |
| (1,1684) | 1:4:A:VAL:HG21  | 1:77:A:ILE:HG12  | 5        | 1.17          |
| (1,1684) | 1:4:A:VAL:HG21  | 1:77:A:ILE:HG13  | 5        | 1.17          |
| (1,1684) | 1:4:A:VAL:HG22  | 1:77:A:ILE:HG12  | 5        | 1.17          |
| (1,1684) | 1:4:A:VAL:HG22  | 1:77:A:ILE:HG13  | 5        | 1.17          |
| (1,1684) | 1:4:A:VAL:HG23  | 1:77:A:ILE:HG12  | 5        | 1.17          |
| (1,1684) | 1:4:A:VAL:HG23  | 1:77:A:ILE:HG13  | 5        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG21  | 1        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 1        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 1        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 1        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 1        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 1        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 1        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 1        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 1        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG21  | 2        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 2        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 2        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 2        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 2        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 2        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 2        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 2        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 2        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG21  | 9        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 9        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 9        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 9        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 9        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 9        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 9        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 9        | 1.17          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 9        | 1.17          |
| (1,822)  | 1:31:A:ALA:H    | 1:32:A:VAL:HG21  | 11       | 1.17          |
| (1,822)  | 1:31:A:ALA:H    | 1:32:A:VAL:HG22  | 11       | 1.17          |
| (1,822)  | 1:31:A:ALA:H    | 1:32:A:VAL:HG23  | 11       | 1.17          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG11  | 1        | 1.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG12  | 1        | 1.17          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG13  | 1        | 1.17          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG11  | 1        | 1.17          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG12  | 1        | 1.17          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG13  | 1        | 1.17          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG11  | 15       | 1.17          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG12  | 15       | 1.17          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG13  | 15       | 1.17          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG11  | 15       | 1.17          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG12  | 15       | 1.17          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG13  | 15       | 1.17          |
| (1,272)  | 1:6:A:PHE:HD1   | 1:4:A:VAL:HG21   | 20       | 1.17          |
| (1,272)  | 1:6:A:PHE:HD1   | 1:4:A:VAL:HG22   | 20       | 1.17          |
| (1,272)  | 1:6:A:PHE:HD1   | 1:4:A:VAL:HG23   | 20       | 1.17          |
| (1,272)  | 1:6:A:PHE:HD2   | 1:4:A:VAL:HG21   | 20       | 1.17          |
| (1,272)  | 1:6:A:PHE:HD2   | 1:4:A:VAL:HG22   | 20       | 1.17          |
| (1,272)  | 1:6:A:PHE:HD2   | 1:4:A:VAL:HG23   | 20       | 1.17          |
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG21 | 1        | 1.16          |
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG22 | 1        | 1.16          |
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG23 | 1        | 1.16          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG21 | 1        | 1.16          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG22 | 1        | 1.16          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG23 | 1        | 1.16          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG21  | 10       | 1.16          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 10       | 1.16          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 10       | 1.16          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 10       | 1.16          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 10       | 1.16          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 10       | 1.16          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 10       | 1.16          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 10       | 1.16          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 10       | 1.16          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG11  | 18       | 1.16          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG12  | 18       | 1.16          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG13  | 18       | 1.16          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG11  | 18       | 1.16          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG12  | 18       | 1.16          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG13  | 18       | 1.16          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD11 | 1        | 1.16          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD12 | 1        | 1.16          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD13 | 1        | 1.16          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD11 | 1        | 1.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 1        | 1.16          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 1        | 1.16          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 1        | 1.16          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 1        | 1.16          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 1        | 1.16          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 5        | 1.16          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 5        | 1.16          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 5        | 1.16          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 5        | 1.16          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 5        | 1.16          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 5        | 1.16          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 5        | 1.16          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 5        | 1.16          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 5        | 1.16          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 9        | 1.16          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 9        | 1.16          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 9        | 1.16          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 9        | 1.16          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 9        | 1.16          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 9        | 1.16          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 4        | 1.15          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 4        | 1.15          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 4        | 1.15          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 4        | 1.15          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 4        | 1.15          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 4        | 1.15          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 10       | 1.15          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 10       | 1.15          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 10       | 1.15          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 10       | 1.15          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 10       | 1.15          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 10       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG21  | 13       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG22  | 13       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG23  | 13       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG21  | 13       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG22  | 13       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG23  | 13       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG21  | 13       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG22  | 13       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG23  | 13       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG21  | 19       | 1.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 19       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 19       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 19       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 19       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 19       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 19       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 19       | 1.15          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 19       | 1.15          |
| (1,911)  | 1:65:A:ILE:HB   | 1:37:A:LEU:HD11  | 7        | 1.15          |
| (1,911)  | 1:65:A:ILE:HB   | 1:37:A:LEU:HD12  | 7        | 1.15          |
| (1,911)  | 1:65:A:ILE:HB   | 1:37:A:LEU:HD13  | 7        | 1.15          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG11  | 8        | 1.15          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG12  | 8        | 1.15          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG13  | 8        | 1.15          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG11  | 8        | 1.15          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG12  | 8        | 1.15          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG13  | 8        | 1.15          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD11 | 4        | 1.15          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD12 | 4        | 1.15          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD13 | 4        | 1.15          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD11 | 4        | 1.15          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD12 | 4        | 1.15          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD13 | 4        | 1.15          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD11 | 4        | 1.15          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD12 | 4        | 1.15          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD13 | 4        | 1.15          |
| (1,516)  | 1:32:A:VAL:HG11 | 1:19:A:GLU:HB2   | 9        | 1.15          |
| (1,516)  | 1:32:A:VAL:HG11 | 1:19:A:GLU:HB3   | 9        | 1.15          |
| (1,516)  | 1:32:A:VAL:HG12 | 1:19:A:GLU:HB2   | 9        | 1.15          |
| (1,516)  | 1:32:A:VAL:HG12 | 1:19:A:GLU:HB3   | 9        | 1.15          |
| (1,516)  | 1:32:A:VAL:HG13 | 1:19:A:GLU:HB2   | 9        | 1.15          |
| (1,516)  | 1:32:A:VAL:HG13 | 1:19:A:GLU:HB3   | 9        | 1.15          |
| (1,370)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG2    | 12       | 1.15          |
| (1,370)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG3    | 12       | 1.15          |
| (1,370)  | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG2    | 12       | 1.15          |
| (1,370)  | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG3    | 12       | 1.15          |
| (1,370)  | 1:37:A:LEU:HD23 | 1:9:A:LYS:HG2    | 12       | 1.15          |
| (1,370)  | 1:37:A:LEU:HD23 | 1:9:A:LYS:HG3    | 12       | 1.15          |
| (1,367)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG2    | 12       | 1.15          |
| (1,367)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG3    | 12       | 1.15          |
| (1,367)  | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG2    | 12       | 1.15          |
| (1,367)  | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG3    | 12       | 1.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 12       | 1.15          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 12       | 1.15          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 8        | 1.15          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 8        | 1.15          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 8        | 1.15          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 20       | 1.15          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 20       | 1.15          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 20       | 1.15          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 20       | 1.15          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 20       | 1.15          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 20       | 1.15          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 20       | 1.15          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 20       | 1.15          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 20       | 1.15          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 20       | 1.15          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 20       | 1.15          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 20       | 1.15          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 14       | 1.14          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 14       | 1.14          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 14       | 1.14          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 14       | 1.14          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 14       | 1.14          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 14       | 1.14          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 14       | 1.14          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 14       | 1.14          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 14       | 1.14          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 20       | 1.14          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 20       | 1.14          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 20       | 1.14          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 20       | 1.14          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 20       | 1.14          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 20       | 1.14          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG21  | 8        | 1.14          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG22  | 8        | 1.14          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG23  | 8        | 1.14          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG21  | 8        | 1.14          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG22  | 8        | 1.14          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG23  | 8        | 1.14          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG21  | 8        | 1.14          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG22  | 8        | 1.14          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG23  | 8        | 1.14          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 3        | 1.14          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,666) | 1:49:A:MET:HE1  | 1:109:A:LEU:HD12 | 3        | 1.14          |
| (1,666) | 1:49:A:MET:HE1  | 1:109:A:LEU:HD13 | 3        | 1.14          |
| (1,666) | 1:49:A:MET:HE2  | 1:109:A:LEU:HD11 | 3        | 1.14          |
| (1,666) | 1:49:A:MET:HE2  | 1:109:A:LEU:HD12 | 3        | 1.14          |
| (1,666) | 1:49:A:MET:HE2  | 1:109:A:LEU:HD13 | 3        | 1.14          |
| (1,666) | 1:49:A:MET:HE3  | 1:109:A:LEU:HD11 | 3        | 1.14          |
| (1,666) | 1:49:A:MET:HE3  | 1:109:A:LEU:HD12 | 3        | 1.14          |
| (1,666) | 1:49:A:MET:HE3  | 1:109:A:LEU:HD13 | 3        | 1.14          |
| (1,666) | 1:49:A:MET:HE1  | 1:109:A:LEU:HD11 | 19       | 1.14          |
| (1,666) | 1:49:A:MET:HE1  | 1:109:A:LEU:HD12 | 19       | 1.14          |
| (1,666) | 1:49:A:MET:HE1  | 1:109:A:LEU:HD13 | 19       | 1.14          |
| (1,666) | 1:49:A:MET:HE2  | 1:109:A:LEU:HD11 | 19       | 1.14          |
| (1,666) | 1:49:A:MET:HE2  | 1:109:A:LEU:HD12 | 19       | 1.14          |
| (1,666) | 1:49:A:MET:HE2  | 1:109:A:LEU:HD13 | 19       | 1.14          |
| (1,666) | 1:49:A:MET:HE3  | 1:109:A:LEU:HD11 | 19       | 1.14          |
| (1,666) | 1:49:A:MET:HE3  | 1:109:A:LEU:HD12 | 19       | 1.14          |
| (1,666) | 1:49:A:MET:HE3  | 1:109:A:LEU:HD13 | 19       | 1.14          |
| (1,666) | 1:49:A:MET:HE1  | 1:109:A:LEU:HD11 | 20       | 1.14          |
| (1,666) | 1:49:A:MET:HE1  | 1:109:A:LEU:HD12 | 20       | 1.14          |
| (1,666) | 1:49:A:MET:HE1  | 1:109:A:LEU:HD13 | 20       | 1.14          |
| (1,666) | 1:49:A:MET:HE2  | 1:109:A:LEU:HD11 | 20       | 1.14          |
| (1,666) | 1:49:A:MET:HE2  | 1:109:A:LEU:HD12 | 20       | 1.14          |
| (1,666) | 1:49:A:MET:HE2  | 1:109:A:LEU:HD13 | 20       | 1.14          |
| (1,666) | 1:49:A:MET:HE3  | 1:109:A:LEU:HD11 | 20       | 1.14          |
| (1,666) | 1:49:A:MET:HE3  | 1:109:A:LEU:HD12 | 20       | 1.14          |
| (1,666) | 1:49:A:MET:HE3  | 1:109:A:LEU:HD13 | 20       | 1.14          |
| (1,370) | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG2    | 3        | 1.14          |
| (1,370) | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG3    | 3        | 1.14          |
| (1,370) | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG2    | 3        | 1.14          |
| (1,370) | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG3    | 3        | 1.14          |
| (1,370) | 1:37:A:LEU:HD23 | 1:9:A:LYS:HG2    | 3        | 1.14          |
| (1,370) | 1:37:A:LEU:HD23 | 1:9:A:LYS:HG3    | 3        | 1.14          |
| (1,367) | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG2    | 3        | 1.14          |
| (1,367) | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG3    | 3        | 1.14          |
| (1,367) | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG2    | 3        | 1.14          |
| (1,367) | 1:37:A:LEU:HD22 | 1:9:A:LYS:HG3    | 3        | 1.14          |
| (1,367) | 1:37:A:LEU:HD23 | 1:9:A:LYS:HG2    | 3        | 1.14          |
| (1,367) | 1:37:A:LEU:HD23 | 1:9:A:LYS:HG3    | 3        | 1.14          |
| (1,272) | 1:6:A:PHE:HD1   | 1:4:A:VAL:HG21   | 14       | 1.14          |
| (1,272) | 1:6:A:PHE:HD1   | 1:4:A:VAL:HG22   | 14       | 1.14          |
| (1,272) | 1:6:A:PHE:HD1   | 1:4:A:VAL:HG23   | 14       | 1.14          |
| (1,272) | 1:6:A:PHE:HD2   | 1:4:A:VAL:HG21   | 14       | 1.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,272)  | 1:6:A:PHE:HD2   | 1:4:A:VAL:HG22   | 14       | 1.14          |
| (1,272)  | 1:6:A:PHE:HD2   | 1:4:A:VAL:HG23   | 14       | 1.14          |
| (1,2908) | 1:32:A:VAL:HG11 | 1:19:A:GLU:H     | 9        | 1.13          |
| (1,2908) | 1:32:A:VAL:HG12 | 1:19:A:GLU:H     | 9        | 1.13          |
| (1,2908) | 1:32:A:VAL:HG13 | 1:19:A:GLU:H     | 9        | 1.13          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD21 | 2        | 1.13          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD22 | 2        | 1.13          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD23 | 2        | 1.13          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD21 | 2        | 1.13          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD22 | 2        | 1.13          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD23 | 2        | 1.13          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD21 | 12       | 1.13          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD22 | 12       | 1.13          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD23 | 12       | 1.13          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD21 | 12       | 1.13          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD22 | 12       | 1.13          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD23 | 12       | 1.13          |
| (1,1684) | 1:4:A:VAL:HG21  | 1:77:A:ILE:HG12  | 1        | 1.13          |
| (1,1684) | 1:4:A:VAL:HG21  | 1:77:A:ILE:HG13  | 1        | 1.13          |
| (1,1684) | 1:4:A:VAL:HG22  | 1:77:A:ILE:HG12  | 1        | 1.13          |
| (1,1684) | 1:4:A:VAL:HG22  | 1:77:A:ILE:HG13  | 1        | 1.13          |
| (1,1684) | 1:4:A:VAL:HG23  | 1:77:A:ILE:HG12  | 1        | 1.13          |
| (1,1684) | 1:4:A:VAL:HG23  | 1:77:A:ILE:HG13  | 1        | 1.13          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG21  | 3        | 1.13          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 3        | 1.13          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 3        | 1.13          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 3        | 1.13          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 3        | 1.13          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 3        | 1.13          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 3        | 1.13          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 3        | 1.13          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 3        | 1.13          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD11 | 16       | 1.13          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD12 | 16       | 1.13          |
| (1,666)  | 1:49:A:MET:HE1  | 1:109:A:LEU:HD13 | 16       | 1.13          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD11 | 16       | 1.13          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD12 | 16       | 1.13          |
| (1,666)  | 1:49:A:MET:HE2  | 1:109:A:LEU:HD13 | 16       | 1.13          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD11 | 16       | 1.13          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD12 | 16       | 1.13          |
| (1,666)  | 1:49:A:MET:HE3  | 1:109:A:LEU:HD13 | 16       | 1.13          |
| (1,370)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG2    | 1        | 1.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 1        | 1.13          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 1        | 1.13          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 1        | 1.13          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 1        | 1.13          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 1        | 1.13          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 8        | 1.13          |
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 8        | 1.13          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 8        | 1.13          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 8        | 1.13          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 8        | 1.13          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 8        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 1        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 1        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 1        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 1        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 1        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 1        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 8        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 8        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 8        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 8        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 8        | 1.13          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 8        | 1.13          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 11       | 1.13          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 11       | 1.13          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 11       | 1.13          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 11       | 1.13          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 11       | 1.13          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 11       | 1.13          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 3        | 1.12          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 3        | 1.12          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 3        | 1.12          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 20       | 1.12          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 20       | 1.12          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 20       | 1.12          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 20       | 1.12          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 20       | 1.12          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 20       | 1.12          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 5        | 1.12          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 5        | 1.12          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 5        | 1.12          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 5        | 1.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2561) | 1:6:A:PHE:HD2   | 1:123:A:VAL:HG12 | 5        | 1.12          |
| (1,2561) | 1:6:A:PHE:HD2   | 1:123:A:VAL:HG13 | 5        | 1.12          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG21  | 12       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 12       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 12       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 12       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 12       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 12       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 12       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 12       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 12       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG21  | 17       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 17       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 17       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 17       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 17       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 17       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 17       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 17       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 17       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG21  | 20       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 20       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 20       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 20       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 20       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 20       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 20       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 20       | 1.12          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 20       | 1.12          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG11  | 2        | 1.12          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG12  | 2        | 1.12          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG13  | 2        | 1.12          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG11  | 2        | 1.12          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG12  | 2        | 1.12          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG13  | 2        | 1.12          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG11  | 14       | 1.12          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG12  | 14       | 1.12          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG13  | 14       | 1.12          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG11  | 14       | 1.12          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG12  | 14       | 1.12          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG13  | 14       | 1.12          |
| (1,516)  | 1:32:A:VAL:HG11 | 1:19:A:GLU:HB2   | 14       | 1.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3   | 14       | 1.12          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2   | 14       | 1.12          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3   | 14       | 1.12          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2   | 14       | 1.12          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3   | 14       | 1.12          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 14       | 1.12          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 14       | 1.12          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 14       | 1.12          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 5        | 1.12          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 5        | 1.12          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 5        | 1.12          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 2        | 1.11          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 2        | 1.11          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 2        | 1.11          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 7        | 1.11          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 7        | 1.11          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 7        | 1.11          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 10       | 1.11          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 10       | 1.11          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 10       | 1.11          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 10       | 1.11          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 10       | 1.11          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 10       | 1.11          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 10       | 1.11          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 10       | 1.11          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 10       | 1.11          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 16       | 1.11          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 16       | 1.11          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 16       | 1.11          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 16       | 1.11          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 16       | 1.11          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 16       | 1.11          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 3        | 1.11          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 3        | 1.11          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 3        | 1.11          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 1        | 1.11          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 1        | 1.11          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 1        | 1.11          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 19       | 1.11          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 19       | 1.11          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 19       | 1.11          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 19       | 1.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 19       | 1.11          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 19       | 1.11          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 19       | 1.11          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 19       | 1.11          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 19       | 1.11          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 19       | 1.11          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 19       | 1.11          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 19       | 1.11          |
| (1,2769) | 1:4:A:VAL:HG21   | 1:30:A:ILE:HB    | 7        | 1.1           |
| (1,2769) | 1:4:A:VAL:HG22   | 1:30:A:ILE:HB    | 7        | 1.1           |
| (1,2769) | 1:4:A:VAL:HG23   | 1:30:A:ILE:HB    | 7        | 1.1           |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 15       | 1.1           |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 15       | 1.1           |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 15       | 1.1           |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 15       | 1.1           |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 15       | 1.1           |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 15       | 1.1           |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 18       | 1.1           |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 18       | 1.1           |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 18       | 1.1           |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 18       | 1.1           |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 18       | 1.1           |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 18       | 1.1           |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 18       | 1.1           |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 18       | 1.1           |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 18       | 1.1           |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 12       | 1.1           |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 12       | 1.1           |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 12       | 1.1           |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG11  | 12       | 1.1           |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG12  | 12       | 1.1           |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG13  | 12       | 1.1           |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG11  | 12       | 1.1           |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG12  | 12       | 1.1           |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG13  | 12       | 1.1           |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 3        | 1.1           |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 3        | 1.1           |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 3        | 1.1           |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 17       | 1.1           |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 17       | 1.1           |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 17       | 1.1           |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 6        | 1.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 6        | 1.1           |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 6        | 1.1           |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 16       | 1.1           |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 16       | 1.1           |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 16       | 1.1           |
| (1,266)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG21   | 6        | 1.1           |
| (1,266)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG22   | 6        | 1.1           |
| (1,266)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG23   | 6        | 1.1           |
| (1,2746) | 1:119:A:VAL:HG21 | 1:15:A:SER:HA    | 1        | 1.09          |
| (1,2746) | 1:119:A:VAL:HG22 | 1:15:A:SER:HA    | 1        | 1.09          |
| (1,2746) | 1:119:A:VAL:HG23 | 1:15:A:SER:HA    | 1        | 1.09          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 8        | 1.09          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 8        | 1.09          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 8        | 1.09          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 8        | 1.09          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 8        | 1.09          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 8        | 1.09          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 12       | 1.09          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 12       | 1.09          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 12       | 1.09          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11  | 14       | 1.09          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12  | 14       | 1.09          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13  | 14       | 1.09          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 2        | 1.09          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 2        | 1.09          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 2        | 1.09          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 2        | 1.09          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 2        | 1.09          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 2        | 1.09          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 2        | 1.09          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 2        | 1.09          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 2        | 1.09          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 9        | 1.09          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 9        | 1.09          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 9        | 1.09          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 9        | 1.09          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 9        | 1.09          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 9        | 1.09          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 9        | 1.09          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 9        | 1.09          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 9        | 1.09          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2   | 20       | 1.09          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3   | 20       | 1.09          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2   | 20       | 1.09          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3   | 20       | 1.09          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2   | 20       | 1.09          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3   | 20       | 1.09          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 10       | 1.09          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 10       | 1.09          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 10       | 1.09          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 14       | 1.09          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 14       | 1.09          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 14       | 1.09          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 4        | 1.09          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 4        | 1.09          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 4        | 1.09          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 4        | 1.09          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 4        | 1.09          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 4        | 1.09          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 19       | 1.09          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 19       | 1.09          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 19       | 1.09          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 19       | 1.09          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 19       | 1.09          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 19       | 1.09          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 15       | 1.08          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 15       | 1.08          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 15       | 1.08          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 20       | 1.08          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 20       | 1.08          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 20       | 1.08          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 20       | 1.08          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 20       | 1.08          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 20       | 1.08          |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG11 | 19       | 1.08          |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG12 | 19       | 1.08          |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG13 | 19       | 1.08          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 3        | 1.08          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 3        | 1.08          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 3        | 1.08          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 3        | 1.08          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 3        | 1.08          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 3        | 1.08          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 11       | 1.08          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG22 | 11       | 1.08          |
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG23 | 11       | 1.08          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG21 | 11       | 1.08          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG22 | 11       | 1.08          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG23 | 11       | 1.08          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD21 | 14       | 1.08          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD22 | 14       | 1.08          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD23 | 14       | 1.08          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD21 | 14       | 1.08          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD22 | 14       | 1.08          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD23 | 14       | 1.08          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG21  | 7        | 1.08          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG22  | 7        | 1.08          |
| (1,1644) | 1:7:A:VAL:HG11  | 1:76:A:VAL:HG23  | 7        | 1.08          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG21  | 7        | 1.08          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG22  | 7        | 1.08          |
| (1,1644) | 1:7:A:VAL:HG12  | 1:76:A:VAL:HG23  | 7        | 1.08          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG21  | 7        | 1.08          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG22  | 7        | 1.08          |
| (1,1644) | 1:7:A:VAL:HG13  | 1:76:A:VAL:HG23  | 7        | 1.08          |
| (1,911)  | 1:65:A:ILE:HB   | 1:37:A:LEU:HD11  | 17       | 1.08          |
| (1,911)  | 1:65:A:ILE:HB   | 1:37:A:LEU:HD12  | 17       | 1.08          |
| (1,911)  | 1:65:A:ILE:HB   | 1:37:A:LEU:HD13  | 17       | 1.08          |
| (1,823)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG21  | 5        | 1.08          |
| (1,823)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG22  | 5        | 1.08          |
| (1,823)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG23  | 5        | 1.08          |
| (1,823)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG21  | 5        | 1.08          |
| (1,823)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG22  | 5        | 1.08          |
| (1,823)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG23  | 5        | 1.08          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG11  | 19       | 1.08          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG12  | 19       | 1.08          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG13  | 19       | 1.08          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG11  | 19       | 1.08          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG12  | 19       | 1.08          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG13  | 19       | 1.08          |
| (1,49)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG2   | 13       | 1.08          |
| (1,49)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG3   | 13       | 1.08          |
| (1,49)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG2   | 13       | 1.08          |
| (1,49)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG3   | 13       | 1.08          |
| (1,49)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG2   | 13       | 1.08          |
| (1,49)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG3   | 13       | 1.08          |
| (1,47)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG2   | 13       | 1.08          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 13       | 1.08          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 13       | 1.08          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 13       | 1.08          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 13       | 1.08          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 13       | 1.08          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 12       | 1.07          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 12       | 1.07          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 12       | 1.07          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 7        | 1.07          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 7        | 1.07          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 7        | 1.07          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 7        | 1.07          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 7        | 1.07          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 7        | 1.07          |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG11 | 20       | 1.07          |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG12 | 20       | 1.07          |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG13 | 20       | 1.07          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 6        | 1.07          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 6        | 1.07          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 6        | 1.07          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 6        | 1.07          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 6        | 1.07          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 6        | 1.07          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 2        | 1.07          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 2        | 1.07          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 2        | 1.07          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 11       | 1.07          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 11       | 1.07          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 11       | 1.07          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 13       | 1.07          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 13       | 1.07          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 13       | 1.07          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 4        | 1.07          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 4        | 1.07          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 4        | 1.07          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 8        | 1.06          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 8        | 1.06          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 8        | 1.06          |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG11 | 1        | 1.06          |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG12 | 1        | 1.06          |
| (1,2412) | 1:120:A:LYS:HA   | 1:119:A:VAL:HG13 | 1        | 1.06          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 7        | 1.06          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 7        | 1.06          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 7        | 1.06          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 7        | 1.06          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 7        | 1.06          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 7        | 1.06          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 7        | 1.06          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 7        | 1.06          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 7        | 1.06          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 17       | 1.06          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 17       | 1.06          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 17       | 1.06          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 17       | 1.06          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22  | 17       | 1.06          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23  | 17       | 1.06          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21  | 17       | 1.06          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22  | 17       | 1.06          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23  | 17       | 1.06          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG11  | 20       | 1.06          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG12  | 20       | 1.06          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG13  | 20       | 1.06          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG11  | 20       | 1.06          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG12  | 20       | 1.06          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG13  | 20       | 1.06          |
| (1,798)  | 1:30:A:ILE:HG12  | 1:32:A:VAL:HG11  | 5        | 1.06          |
| (1,798)  | 1:30:A:ILE:HG12  | 1:32:A:VAL:HG12  | 5        | 1.06          |
| (1,798)  | 1:30:A:ILE:HG12  | 1:32:A:VAL:HG13  | 5        | 1.06          |
| (1,798)  | 1:30:A:ILE:HG13  | 1:32:A:VAL:HG11  | 5        | 1.06          |
| (1,798)  | 1:30:A:ILE:HG13  | 1:32:A:VAL:HG12  | 5        | 1.06          |
| (1,798)  | 1:30:A:ILE:HG13  | 1:32:A:VAL:HG13  | 5        | 1.06          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 17       | 1.06          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 17       | 1.06          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 17       | 1.06          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 17       | 1.06          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 17       | 1.06          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 17       | 1.06          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 17       | 1.06          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 17       | 1.06          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 17       | 1.06          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 1        | 1.06          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 1        | 1.06          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 1        | 1.06          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2   | 15       | 1.06          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3   | 15       | 1.06          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2   | 15       | 1.06          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3   | 15       | 1.06          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2   | 15       | 1.06          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3   | 15       | 1.06          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11  | 8        | 1.05          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12  | 8        | 1.05          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13  | 8        | 1.05          |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG11 | 19       | 1.05          |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG12 | 19       | 1.05          |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG13 | 19       | 1.05          |
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG11 | 19       | 1.05          |
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG12 | 19       | 1.05          |
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG13 | 19       | 1.05          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 3        | 1.05          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 3        | 1.05          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 3        | 1.05          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 3        | 1.05          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 3        | 1.05          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 3        | 1.05          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG21  | 6        | 1.05          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG22  | 6        | 1.05          |
| (1,1644) | 1:7:A:VAL:HG11   | 1:76:A:VAL:HG23  | 6        | 1.05          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG21  | 6        | 1.05          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG22  | 6        | 1.05          |
| (1,1644) | 1:7:A:VAL:HG12   | 1:76:A:VAL:HG23  | 6        | 1.05          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG21  | 6        | 1.05          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG22  | 6        | 1.05          |
| (1,1644) | 1:7:A:VAL:HG13   | 1:76:A:VAL:HG23  | 6        | 1.05          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG11  | 3        | 1.05          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG12  | 3        | 1.05          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG13  | 3        | 1.05          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG11  | 3        | 1.05          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG12  | 3        | 1.05          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG13  | 3        | 1.05          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2   | 3        | 1.05          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3   | 3        | 1.05          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2   | 3        | 1.05          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3   | 3        | 1.05          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2   | 3        | 1.05          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3   | 3        | 1.05          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 2        | 1.05          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 2        | 1.05          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 2        | 1.05          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 6        | 1.05          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 6        | 1.05          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 6        | 1.05          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 12       | 1.05          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 12       | 1.05          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 12       | 1.05          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 18       | 1.05          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 18       | 1.05          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 18       | 1.05          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 19       | 1.05          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 19       | 1.05          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 19       | 1.05          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 12       | 1.05          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 12       | 1.05          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 12       | 1.05          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 12       | 1.05          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 12       | 1.05          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 12       | 1.05          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG11 | 12       | 1.04          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG12 | 12       | 1.04          |
| (1,2317) | 1:111:A:VAL:HG21 | 1:115:A:VAL:HG13 | 12       | 1.04          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG11 | 12       | 1.04          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG12 | 12       | 1.04          |
| (1,2317) | 1:111:A:VAL:HG22 | 1:115:A:VAL:HG13 | 12       | 1.04          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG11 | 12       | 1.04          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG12 | 12       | 1.04          |
| (1,2317) | 1:111:A:VAL:HG23 | 1:115:A:VAL:HG13 | 12       | 1.04          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 12       | 1.04          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 12       | 1.04          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 12       | 1.04          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 12       | 1.04          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 12       | 1.04          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 12       | 1.04          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 12       | 1.04          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 12       | 1.04          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 12       | 1.04          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 7        | 1.04          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 7        | 1.04          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 7        | 1.04          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 8        | 1.04          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 8        | 1.04          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 8        | 1.04          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 15       | 1.04          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 15       | 1.04          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 15       | 1.04          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 20       | 1.04          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 20       | 1.04          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 20       | 1.04          |
| (1,244)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HB     | 6        | 1.04          |
| (1,244)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HB     | 6        | 1.04          |
| (1,244)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HB     | 6        | 1.04          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 10       | 1.04          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 10       | 1.04          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 10       | 1.04          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 18       | 1.03          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 18       | 1.03          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 18       | 1.03          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 18       | 1.03          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 18       | 1.03          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 18       | 1.03          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 14       | 1.03          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 14       | 1.03          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 14       | 1.03          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11  | 6        | 1.03          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12  | 6        | 1.03          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13  | 6        | 1.03          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 10       | 1.03          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 10       | 1.03          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 10       | 1.03          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 8        | 1.03          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 8        | 1.03          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 8        | 1.03          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 8        | 1.03          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 8        | 1.03          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 8        | 1.03          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 8        | 1.03          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 8        | 1.03          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 8        | 1.03          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 5        | 1.03          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 5        | 1.03          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 5        | 1.03          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 15       | 1.03          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 15       | 1.03          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 15       | 1.03          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 15       | 1.03          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 15       | 1.03          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 15       | 1.03          |
| (1,144)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HZ     | 7        | 1.03          |
| (1,144)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HZ     | 7        | 1.03          |
| (1,144)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HZ     | 7        | 1.03          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 1        | 1.02          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 1        | 1.02          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 1        | 1.02          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 1        | 1.02          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 1        | 1.02          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 1        | 1.02          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 5        | 1.02          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 5        | 1.02          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 5        | 1.02          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 5        | 1.02          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 5        | 1.02          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 5        | 1.02          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 16       | 1.02          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 16       | 1.02          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 16       | 1.02          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 16       | 1.02          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22  | 16       | 1.02          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23  | 16       | 1.02          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21  | 16       | 1.02          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22  | 16       | 1.02          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23  | 16       | 1.02          |
| (1,1898) | 1:91:A:VAL:HG11  | 1:92:A:THR:HG21  | 10       | 1.02          |
| (1,1898) | 1:91:A:VAL:HG11  | 1:92:A:THR:HG22  | 10       | 1.02          |
| (1,1898) | 1:91:A:VAL:HG11  | 1:92:A:THR:HG23  | 10       | 1.02          |
| (1,1898) | 1:91:A:VAL:HG12  | 1:92:A:THR:HG21  | 10       | 1.02          |
| (1,1898) | 1:91:A:VAL:HG12  | 1:92:A:THR:HG22  | 10       | 1.02          |
| (1,1898) | 1:91:A:VAL:HG12  | 1:92:A:THR:HG23  | 10       | 1.02          |
| (1,1898) | 1:91:A:VAL:HG13  | 1:92:A:THR:HG21  | 10       | 1.02          |
| (1,1898) | 1:91:A:VAL:HG13  | 1:92:A:THR:HG22  | 10       | 1.02          |
| (1,1898) | 1:91:A:VAL:HG13  | 1:92:A:THR:HG23  | 10       | 1.02          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 8        | 1.02          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 8        | 1.02          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 8        | 1.02          |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA    | 17       | 1.02          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1776) | 1:37:A:LEU:HD12  | 1:86:A:LEU:HA    | 17       | 1.02          |
| (1,1776) | 1:37:A:LEU:HD13  | 1:86:A:LEU:HA    | 17       | 1.02          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD11  | 17       | 1.02          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12  | 17       | 1.02          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13  | 17       | 1.02          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 16       | 1.02          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 16       | 1.02          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 16       | 1.02          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 1        | 1.02          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 1        | 1.02          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 1        | 1.02          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 1        | 1.02          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 1        | 1.02          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 1        | 1.02          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 2        | 1.02          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 2        | 1.02          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 2        | 1.02          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 2        | 1.02          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 2        | 1.02          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 2        | 1.02          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 16       | 1.02          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 16       | 1.02          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 16       | 1.02          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 16       | 1.02          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 16       | 1.02          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 16       | 1.02          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 16       | 1.02          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 16       | 1.02          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 16       | 1.02          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 16       | 1.02          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 16       | 1.02          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 16       | 1.02          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD11  | 17       | 1.02          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD12  | 17       | 1.02          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD13  | 17       | 1.02          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 15       | 1.01          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 15       | 1.01          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 15       | 1.01          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 15       | 1.01          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 15       | 1.01          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 15       | 1.01          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 8        | 1.01          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 8        | 1.01          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 8        | 1.01          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 8        | 1.01          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 8        | 1.01          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 8        | 1.01          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 2        | 1.01          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 2        | 1.01          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 2        | 1.01          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 2        | 1.01          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22  | 2        | 1.01          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23  | 2        | 1.01          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21  | 2        | 1.01          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22  | 2        | 1.01          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23  | 2        | 1.01          |
| (1,845)  | 1:79:A:LEU:HD11  | 1:34:A:SER:HA    | 8        | 1.01          |
| (1,845)  | 1:79:A:LEU:HD12  | 1:34:A:SER:HA    | 8        | 1.01          |
| (1,845)  | 1:79:A:LEU:HD13  | 1:34:A:SER:HA    | 8        | 1.01          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2   | 19       | 1.01          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3   | 19       | 1.01          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2   | 19       | 1.01          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3   | 19       | 1.01          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2   | 19       | 1.01          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3   | 19       | 1.01          |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 4        | 1.01          |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 4        | 1.01          |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 4        | 1.01          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 9        | 1.01          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 9        | 1.01          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 9        | 1.01          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11   | 18       | 1.01          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12   | 18       | 1.01          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13   | 18       | 1.01          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11   | 18       | 1.01          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12   | 18       | 1.01          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13   | 18       | 1.01          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 3        | 1.01          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 3        | 1.01          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 3        | 1.01          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 18       | 1.01          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 18       | 1.01          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 18       | 1.01          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H    | 3        | 1.0           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H    | 3        | 1.0           |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H    | 3        | 1.0           |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 2        | 1.0           |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 2        | 1.0           |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 2        | 1.0           |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 2        | 1.0           |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 2        | 1.0           |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 2        | 1.0           |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21  | 7        | 1.0           |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22  | 7        | 1.0           |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23  | 7        | 1.0           |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21  | 7        | 1.0           |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22  | 7        | 1.0           |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23  | 7        | 1.0           |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21  | 7        | 1.0           |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22  | 7        | 1.0           |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23  | 7        | 1.0           |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 18       | 1.0           |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 18       | 1.0           |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 18       | 1.0           |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 18       | 1.0           |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 18       | 1.0           |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 18       | 1.0           |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 18       | 1.0           |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 18       | 1.0           |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 18       | 1.0           |
| (1,347)  | 1:111:A:VAL:HG21 | 1:112:A:PHE:HA   | 9        | 1.0           |
| (1,347)  | 1:111:A:VAL:HG22 | 1:112:A:PHE:HA   | 9        | 1.0           |
| (1,347)  | 1:111:A:VAL:HG23 | 1:112:A:PHE:HA   | 9        | 1.0           |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 10       | 1.0           |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 10       | 1.0           |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 10       | 1.0           |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 10       | 1.0           |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 10       | 1.0           |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 10       | 1.0           |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ     | 7        | 1.0           |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ     | 7        | 1.0           |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ     | 7        | 1.0           |
| (1,144)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HZ     | 16       | 1.0           |
| (1,144)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HZ     | 16       | 1.0           |
| (1,144)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HZ     | 16       | 1.0           |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 12       | 1.0           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 12       | 1.0           |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 12       | 1.0           |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 12       | 1.0           |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 12       | 1.0           |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 12       | 1.0           |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 12       | 1.0           |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 12       | 1.0           |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 12       | 1.0           |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 12       | 1.0           |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 12       | 1.0           |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 12       | 1.0           |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 10       | 0.99          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 10       | 0.99          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 10       | 0.99          |
| (1,2746) | 1:119:A:VAL:HG21 | 1:15:A:SER:HA    | 20       | 0.99          |
| (1,2746) | 1:119:A:VAL:HG22 | 1:15:A:SER:HA    | 20       | 0.99          |
| (1,2746) | 1:119:A:VAL:HG23 | 1:15:A:SER:HA    | 20       | 0.99          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 12       | 0.99          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 12       | 0.99          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 12       | 0.99          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 12       | 0.99          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 12       | 0.99          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 12       | 0.99          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 19       | 0.99          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 19       | 0.99          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 19       | 0.99          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 19       | 0.99          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 19       | 0.99          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 19       | 0.99          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 12       | 0.99          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 12       | 0.99          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 12       | 0.99          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 12       | 0.99          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 12       | 0.99          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 12       | 0.99          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 18       | 0.99          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 18       | 0.99          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 18       | 0.99          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 18       | 0.99          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 18       | 0.99          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 18       | 0.99          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD21 | 19       | 0.99          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD22 | 19       | 0.99          |
| (1,2206) | 1:112:A:PHE:HD1  | 1:109:A:LEU:HD23 | 19       | 0.99          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD21 | 19       | 0.99          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD22 | 19       | 0.99          |
| (1,2206) | 1:112:A:PHE:HD2  | 1:109:A:LEU:HD23 | 19       | 0.99          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 17       | 0.99          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 17       | 0.99          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 17       | 0.99          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 17       | 0.99          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 17       | 0.99          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 17       | 0.99          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 17       | 0.99          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 17       | 0.99          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 17       | 0.99          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 17       | 0.99          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 17       | 0.99          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 17       | 0.99          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11  | 11       | 0.99          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12  | 11       | 0.99          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13  | 11       | 0.99          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG11  | 16       | 0.99          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG12  | 16       | 0.99          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG13  | 16       | 0.99          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG11  | 16       | 0.99          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG12  | 16       | 0.99          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG13  | 16       | 0.99          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21   | 10       | 0.99          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22   | 10       | 0.99          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23   | 10       | 0.99          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 3        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 3        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 3        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 3        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 3        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 3        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 5        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 5        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 5        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 5        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 5        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 5        | 0.99          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 16       | 0.99          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 16       | 0.99          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 16       | 0.99          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 16       | 0.99          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 16       | 0.99          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 16       | 0.99          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 6        | 0.98          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 6        | 0.98          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 6        | 0.98          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 6        | 0.98          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 6        | 0.98          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 6        | 0.98          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 6        | 0.98          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 6        | 0.98          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 6        | 0.98          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 6        | 0.98          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 6        | 0.98          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 6        | 0.98          |
| (1,2084) | 1:79:A:LEU:HD21  | 1:101:A:LEU:HG   | 16       | 0.98          |
| (1,2084) | 1:79:A:LEU:HD22  | 1:101:A:LEU:HG   | 16       | 0.98          |
| (1,2084) | 1:79:A:LEU:HD23  | 1:101:A:LEU:HG   | 16       | 0.98          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2   | 17       | 0.98          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3   | 17       | 0.98          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2   | 17       | 0.98          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3   | 17       | 0.98          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2   | 17       | 0.98          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3   | 17       | 0.98          |
| (1,244)  | 1:32:A:VAL:HG21  | 1:4:A:VAL:HB     | 13       | 0.98          |
| (1,244)  | 1:32:A:VAL:HG22  | 1:4:A:VAL:HB     | 13       | 0.98          |
| (1,244)  | 1:32:A:VAL:HG23  | 1:4:A:VAL:HB     | 13       | 0.98          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 7        | 0.98          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 7        | 0.98          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 7        | 0.98          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 7        | 0.98          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 7        | 0.98          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 7        | 0.98          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 8        | 0.98          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 8        | 0.98          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 8        | 0.98          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 8        | 0.98          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 8        | 0.98          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 8        | 0.98          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 7        | 0.98          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,47)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG3   | 7        | 0.98          |
| (1,47)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG2   | 7        | 0.98          |
| (1,47)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG3   | 7        | 0.98          |
| (1,47)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG2   | 7        | 0.98          |
| (1,47)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG3   | 7        | 0.98          |
| (1,47)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG2   | 8        | 0.98          |
| (1,47)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG3   | 8        | 0.98          |
| (1,47)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG2   | 8        | 0.98          |
| (1,47)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG3   | 8        | 0.98          |
| (1,47)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG2   | 8        | 0.98          |
| (1,47)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG3   | 8        | 0.98          |
| (1,3349) | 1:4:A:VAL:HG21  | 1:77:A:ILE:H     | 11       | 0.97          |
| (1,3349) | 1:4:A:VAL:HG22  | 1:77:A:ILE:H     | 11       | 0.97          |
| (1,3349) | 1:4:A:VAL:HG23  | 1:77:A:ILE:H     | 11       | 0.97          |
| (1,2908) | 1:32:A:VAL:HG11 | 1:19:A:GLU:H     | 18       | 0.97          |
| (1,2908) | 1:32:A:VAL:HG12 | 1:19:A:GLU:H     | 18       | 0.97          |
| (1,2908) | 1:32:A:VAL:HG13 | 1:19:A:GLU:H     | 18       | 0.97          |
| (1,2561) | 1:6:A:PHE:HD1   | 1:123:A:VAL:HG11 | 17       | 0.97          |
| (1,2561) | 1:6:A:PHE:HD1   | 1:123:A:VAL:HG12 | 17       | 0.97          |
| (1,2561) | 1:6:A:PHE:HD1   | 1:123:A:VAL:HG13 | 17       | 0.97          |
| (1,2561) | 1:6:A:PHE:HD2   | 1:123:A:VAL:HG11 | 17       | 0.97          |
| (1,2561) | 1:6:A:PHE:HD2   | 1:123:A:VAL:HG12 | 17       | 0.97          |
| (1,2561) | 1:6:A:PHE:HD2   | 1:123:A:VAL:HG13 | 17       | 0.97          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD21 | 1        | 0.97          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD22 | 1        | 0.97          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD23 | 1        | 0.97          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD21 | 1        | 0.97          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD22 | 1        | 0.97          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD23 | 1        | 0.97          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG11  | 17       | 0.97          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG12  | 17       | 0.97          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG13  | 17       | 0.97          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG11  | 17       | 0.97          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG12  | 17       | 0.97          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG13  | 17       | 0.97          |
| (1,516)  | 1:32:A:VAL:HG11 | 1:19:A:GLU:HB2   | 2        | 0.97          |
| (1,516)  | 1:32:A:VAL:HG11 | 1:19:A:GLU:HB3   | 2        | 0.97          |
| (1,516)  | 1:32:A:VAL:HG12 | 1:19:A:GLU:HB2   | 2        | 0.97          |
| (1,516)  | 1:32:A:VAL:HG12 | 1:19:A:GLU:HB3   | 2        | 0.97          |
| (1,516)  | 1:32:A:VAL:HG13 | 1:19:A:GLU:HB2   | 2        | 0.97          |
| (1,516)  | 1:32:A:VAL:HG13 | 1:19:A:GLU:HB3   | 2        | 0.97          |
| (1,370)  | 1:37:A:LEU:HD21 | 1:9:A:LYS:HG2    | 7        | 0.97          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,370)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 7        | 0.97          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 7        | 0.97          |
| (1,370)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 7        | 0.97          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 7        | 0.97          |
| (1,370)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 7        | 0.97          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG2    | 7        | 0.97          |
| (1,367)  | 1:37:A:LEU:HD21  | 1:9:A:LYS:HG3    | 7        | 0.97          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG2    | 7        | 0.97          |
| (1,367)  | 1:37:A:LEU:HD22  | 1:9:A:LYS:HG3    | 7        | 0.97          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG2    | 7        | 0.97          |
| (1,367)  | 1:37:A:LEU:HD23  | 1:9:A:LYS:HG3    | 7        | 0.97          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 5        | 0.97          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 5        | 0.97          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 5        | 0.97          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11   | 5        | 0.97          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12   | 5        | 0.97          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13   | 5        | 0.97          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11   | 5        | 0.97          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12   | 5        | 0.97          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13   | 5        | 0.97          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21   | 11       | 0.97          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22   | 11       | 0.97          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23   | 11       | 0.97          |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG11   | 6        | 0.97          |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG12   | 6        | 0.97          |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG13   | 6        | 0.97          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 15       | 0.97          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 15       | 0.97          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 15       | 0.97          |
| (1,144)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HZ     | 9        | 0.97          |
| (1,144)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HZ     | 9        | 0.97          |
| (1,144)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HZ     | 9        | 0.97          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 2        | 0.96          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 2        | 0.96          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 2        | 0.96          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 2        | 0.96          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 2        | 0.96          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 2        | 0.96          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 4        | 0.96          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 4        | 0.96          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 4        | 0.96          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 4        | 0.96          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA  | 4        | 0.96          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA  | 4        | 0.96          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21 | 3        | 0.96          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22 | 3        | 0.96          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23 | 3        | 0.96          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21 | 3        | 0.96          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22 | 3        | 0.96          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23 | 3        | 0.96          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21 | 3        | 0.96          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22 | 3        | 0.96          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23 | 3        | 0.96          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11 | 4        | 0.96          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12 | 4        | 0.96          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13 | 4        | 0.96          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11 | 4        | 0.96          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12 | 4        | 0.96          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13 | 4        | 0.96          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 17       | 0.96          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 17       | 0.96          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 17       | 0.96          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG11 | 9        | 0.96          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG12 | 9        | 0.96          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG13 | 9        | 0.96          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG11 | 9        | 0.96          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG12 | 9        | 0.96          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG13 | 9        | 0.96          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2  | 11       | 0.96          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3  | 11       | 0.96          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2  | 11       | 0.96          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3  | 11       | 0.96          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2  | 11       | 0.96          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3  | 11       | 0.96          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2  | 11       | 0.96          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3  | 11       | 0.96          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2  | 11       | 0.96          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3  | 11       | 0.96          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2  | 11       | 0.96          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3  | 11       | 0.96          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H   | 6        | 0.95          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H   | 6        | 0.95          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H   | 6        | 0.95          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H   | 13       | 0.95          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H    | 13       | 0.95          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H    | 13       | 0.95          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11  | 18       | 0.95          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12  | 18       | 0.95          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13  | 18       | 0.95          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 17       | 0.95          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 17       | 0.95          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 17       | 0.95          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 17       | 0.95          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 17       | 0.95          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 17       | 0.95          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 18       | 0.95          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 18       | 0.95          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 18       | 0.95          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 18       | 0.95          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 18       | 0.95          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 18       | 0.95          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG11  | 10       | 0.95          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG12  | 10       | 0.95          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG13  | 10       | 0.95          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG11  | 10       | 0.95          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG12  | 10       | 0.95          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG13  | 10       | 0.95          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG21   | 18       | 0.95          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG22   | 18       | 0.95          |
| (1,272)  | 1:6:A:PHE:HD1    | 1:4:A:VAL:HG23   | 18       | 0.95          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG21   | 18       | 0.95          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG22   | 18       | 0.95          |
| (1,272)  | 1:6:A:PHE:HD2    | 1:4:A:VAL:HG23   | 18       | 0.95          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 19       | 0.95          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 19       | 0.95          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 19       | 0.95          |
| (1,2744) | 1:79:A:LEU:HD11  | 1:15:A:SER:HA    | 16       | 0.94          |
| (1,2744) | 1:79:A:LEU:HD12  | 1:15:A:SER:HA    | 16       | 0.94          |
| (1,2744) | 1:79:A:LEU:HD13  | 1:15:A:SER:HA    | 16       | 0.94          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 2        | 0.94          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 2        | 0.94          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 2        | 0.94          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 2        | 0.94          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 2        | 0.94          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 2        | 0.94          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 12       | 0.94          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 12       | 0.94          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 12       | 0.94          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 12       | 0.94          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 12       | 0.94          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 12       | 0.94          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD11  | 16       | 0.94          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD12  | 16       | 0.94          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD13  | 16       | 0.94          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD11 | 7        | 0.94          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD12 | 7        | 0.94          |
| (1,666)  | 1:49:A:MET:HE1   | 1:109:A:LEU:HD13 | 7        | 0.94          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD11 | 7        | 0.94          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD12 | 7        | 0.94          |
| (1,666)  | 1:49:A:MET:HE2   | 1:109:A:LEU:HD13 | 7        | 0.94          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD11 | 7        | 0.94          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD12 | 7        | 0.94          |
| (1,666)  | 1:49:A:MET:HE3   | 1:109:A:LEU:HD13 | 7        | 0.94          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 16       | 0.94          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 16       | 0.94          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 16       | 0.94          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 12       | 0.93          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 12       | 0.93          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 12       | 0.93          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 14       | 0.93          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 14       | 0.93          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 14       | 0.93          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 20       | 0.93          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 20       | 0.93          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 20       | 0.93          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 19       | 0.93          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 19       | 0.93          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 19       | 0.93          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 19       | 0.93          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22  | 19       | 0.93          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23  | 19       | 0.93          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21  | 19       | 0.93          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22  | 19       | 0.93          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23  | 19       | 0.93          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11  | 3        | 0.93          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12  | 3        | 0.93          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13  | 3        | 0.93          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 10       | 0.93          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,323)  | 1:86:A:LEU:HA   | 1:7:A:VAL:HG22   | 10       | 0.93          |
| (1,323)  | 1:86:A:LEU:HA   | 1:7:A:VAL:HG23   | 10       | 0.93          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG21   | 12       | 0.93          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG22   | 12       | 0.93          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG23   | 12       | 0.93          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG21   | 14       | 0.93          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG22   | 14       | 0.93          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG23   | 14       | 0.93          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG21   | 20       | 0.93          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG22   | 20       | 0.93          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG23   | 20       | 0.93          |
| (1,60)   | 1:79:A:LEU:HD11 | 1:78:A:SER:H     | 9        | 0.93          |
| (1,60)   | 1:79:A:LEU:HD12 | 1:78:A:SER:H     | 9        | 0.93          |
| (1,60)   | 1:79:A:LEU:HD13 | 1:78:A:SER:H     | 9        | 0.93          |
| (1,3349) | 1:4:A:VAL:HG21  | 1:77:A:ILE:H     | 19       | 0.92          |
| (1,3349) | 1:4:A:VAL:HG22  | 1:77:A:ILE:H     | 19       | 0.92          |
| (1,3349) | 1:4:A:VAL:HG23  | 1:77:A:ILE:H     | 19       | 0.92          |
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG21 | 6        | 0.92          |
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG22 | 6        | 0.92          |
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG23 | 6        | 0.92          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG21 | 6        | 0.92          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG22 | 6        | 0.92          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG23 | 6        | 0.92          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD21 | 20       | 0.92          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD22 | 20       | 0.92          |
| (1,2206) | 1:112:A:PHE:HD1 | 1:109:A:LEU:HD23 | 20       | 0.92          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD21 | 20       | 0.92          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD22 | 20       | 0.92          |
| (1,2206) | 1:112:A:PHE:HD2 | 1:109:A:LEU:HD23 | 20       | 0.92          |
| (1,1898) | 1:91:A:VAL:HG11 | 1:92:A:THR:HG21  | 11       | 0.92          |
| (1,1898) | 1:91:A:VAL:HG11 | 1:92:A:THR:HG22  | 11       | 0.92          |
| (1,1898) | 1:91:A:VAL:HG11 | 1:92:A:THR:HG23  | 11       | 0.92          |
| (1,1898) | 1:91:A:VAL:HG12 | 1:92:A:THR:HG21  | 11       | 0.92          |
| (1,1898) | 1:91:A:VAL:HG12 | 1:92:A:THR:HG22  | 11       | 0.92          |
| (1,1898) | 1:91:A:VAL:HG12 | 1:92:A:THR:HG23  | 11       | 0.92          |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG21  | 11       | 0.92          |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG22  | 11       | 0.92          |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG23  | 11       | 0.92          |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG11  | 10       | 0.92          |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG12  | 10       | 0.92          |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG13  | 10       | 0.92          |
| (1,1597) | 1:4:A:VAL:HG21  | 1:75:A:VAL:HG11  | 6        | 0.92          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1597) | 1:4:A:VAL:HG21   | 1:75:A:VAL:HG12 | 6        | 0.92          |
| (1,1597) | 1:4:A:VAL:HG21   | 1:75:A:VAL:HG13 | 6        | 0.92          |
| (1,1597) | 1:4:A:VAL:HG22   | 1:75:A:VAL:HG11 | 6        | 0.92          |
| (1,1597) | 1:4:A:VAL:HG22   | 1:75:A:VAL:HG12 | 6        | 0.92          |
| (1,1597) | 1:4:A:VAL:HG22   | 1:75:A:VAL:HG13 | 6        | 0.92          |
| (1,1597) | 1:4:A:VAL:HG23   | 1:75:A:VAL:HG11 | 6        | 0.92          |
| (1,1597) | 1:4:A:VAL:HG23   | 1:75:A:VAL:HG12 | 6        | 0.92          |
| (1,1597) | 1:4:A:VAL:HG23   | 1:75:A:VAL:HG13 | 6        | 0.92          |
| (1,845)  | 1:79:A:LEU:HD11  | 1:34:A:SER:HA   | 18       | 0.92          |
| (1,845)  | 1:79:A:LEU:HD12  | 1:34:A:SER:HA   | 18       | 0.92          |
| (1,845)  | 1:79:A:LEU:HD13  | 1:34:A:SER:HA   | 18       | 0.92          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21  | 19       | 0.92          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22  | 19       | 0.92          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23  | 19       | 0.92          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2 | 5        | 0.91          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3 | 5        | 0.91          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2 | 5        | 0.91          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3 | 5        | 0.91          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2 | 5        | 0.91          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3 | 5        | 0.91          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21 | 11       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22 | 11       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23 | 11       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21 | 11       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22 | 11       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23 | 11       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21 | 11       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22 | 11       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23 | 11       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21 | 20       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22 | 20       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23 | 20       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21 | 20       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22 | 20       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23 | 20       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21 | 20       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22 | 20       | 0.91          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23 | 20       | 0.91          |
| (1,1898) | 1:91:A:VAL:HG11  | 1:92:A:THR:HG21 | 9        | 0.91          |
| (1,1898) | 1:91:A:VAL:HG11  | 1:92:A:THR:HG22 | 9        | 0.91          |
| (1,1898) | 1:91:A:VAL:HG11  | 1:92:A:THR:HG23 | 9        | 0.91          |
| (1,1898) | 1:91:A:VAL:HG12  | 1:92:A:THR:HG21 | 9        | 0.91          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1898) | 1:91:A:VAL:HG12 | 1:92:A:THR:HG22 | 9        | 0.91          |
| (1,1898) | 1:91:A:VAL:HG12 | 1:92:A:THR:HG23 | 9        | 0.91          |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG21 | 9        | 0.91          |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG22 | 9        | 0.91          |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG23 | 9        | 0.91          |
| (1,1898) | 1:91:A:VAL:HG11 | 1:92:A:THR:HG21 | 16       | 0.91          |
| (1,1898) | 1:91:A:VAL:HG11 | 1:92:A:THR:HG22 | 16       | 0.91          |
| (1,1898) | 1:91:A:VAL:HG11 | 1:92:A:THR:HG23 | 16       | 0.91          |
| (1,1898) | 1:91:A:VAL:HG12 | 1:92:A:THR:HG21 | 16       | 0.91          |
| (1,1898) | 1:91:A:VAL:HG12 | 1:92:A:THR:HG22 | 16       | 0.91          |
| (1,1898) | 1:91:A:VAL:HG12 | 1:92:A:THR:HG23 | 16       | 0.91          |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG21 | 16       | 0.91          |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG22 | 16       | 0.91          |
| (1,1898) | 1:91:A:VAL:HG13 | 1:92:A:THR:HG23 | 16       | 0.91          |
| (1,1244) | 1:21:A:PHE:HD1  | 1:53:A:VAL:HG11 | 2        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD1  | 1:53:A:VAL:HG12 | 2        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD1  | 1:53:A:VAL:HG13 | 2        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD2  | 1:53:A:VAL:HG11 | 2        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD2  | 1:53:A:VAL:HG12 | 2        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD2  | 1:53:A:VAL:HG13 | 2        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD1  | 1:53:A:VAL:HG11 | 6        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD1  | 1:53:A:VAL:HG12 | 6        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD1  | 1:53:A:VAL:HG13 | 6        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD2  | 1:53:A:VAL:HG11 | 6        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD2  | 1:53:A:VAL:HG12 | 6        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD2  | 1:53:A:VAL:HG13 | 6        | 0.91          |
| (1,1244) | 1:21:A:PHE:HD1  | 1:53:A:VAL:HG11 | 20       | 0.91          |
| (1,1244) | 1:21:A:PHE:HD1  | 1:53:A:VAL:HG12 | 20       | 0.91          |
| (1,1244) | 1:21:A:PHE:HD1  | 1:53:A:VAL:HG13 | 20       | 0.91          |
| (1,1244) | 1:21:A:PHE:HD2  | 1:53:A:VAL:HG11 | 20       | 0.91          |
| (1,1244) | 1:21:A:PHE:HD2  | 1:53:A:VAL:HG12 | 20       | 0.91          |
| (1,1244) | 1:21:A:PHE:HD2  | 1:53:A:VAL:HG13 | 20       | 0.91          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG11 | 6        | 0.91          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG12 | 6        | 0.91          |
| (1,799)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG13 | 6        | 0.91          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG11 | 6        | 0.91          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG12 | 6        | 0.91          |
| (1,799)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG13 | 6        | 0.91          |
| (1,271)  | 1:6:A:PHE:HE1   | 1:4:A:VAL:HG21  | 9        | 0.91          |
| (1,271)  | 1:6:A:PHE:HE1   | 1:4:A:VAL:HG22  | 9        | 0.91          |
| (1,271)  | 1:6:A:PHE:HE1   | 1:4:A:VAL:HG23  | 9        | 0.91          |
| (1,271)  | 1:6:A:PHE:HE2   | 1:4:A:VAL:HG21  | 9        | 0.91          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22  | 9        | 0.91          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23  | 9        | 0.91          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H    | 15       | 0.9           |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H    | 15       | 0.9           |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H    | 15       | 0.9           |
| (1,3025) | 1:32:A:VAL:HG11  | 1:34:A:SER:H    | 9        | 0.9           |
| (1,3025) | 1:32:A:VAL:HG12  | 1:34:A:SER:H    | 9        | 0.9           |
| (1,3025) | 1:32:A:VAL:HG13  | 1:34:A:SER:H    | 9        | 0.9           |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H    | 11       | 0.9           |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H    | 11       | 0.9           |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H    | 11       | 0.9           |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11 | 10       | 0.9           |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12 | 10       | 0.9           |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13 | 10       | 0.9           |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2 | 12       | 0.9           |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3 | 12       | 0.9           |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2 | 12       | 0.9           |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3 | 12       | 0.9           |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2 | 12       | 0.9           |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3 | 12       | 0.9           |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21 | 15       | 0.9           |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22 | 15       | 0.9           |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23 | 15       | 0.9           |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21 | 15       | 0.9           |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22 | 15       | 0.9           |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23 | 15       | 0.9           |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21 | 15       | 0.9           |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22 | 15       | 0.9           |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23 | 15       | 0.9           |
| (1,1898) | 1:91:A:VAL:HG11  | 1:92:A:THR:HG21 | 8        | 0.9           |
| (1,1898) | 1:91:A:VAL:HG11  | 1:92:A:THR:HG22 | 8        | 0.9           |
| (1,1898) | 1:91:A:VAL:HG11  | 1:92:A:THR:HG23 | 8        | 0.9           |
| (1,1898) | 1:91:A:VAL:HG12  | 1:92:A:THR:HG21 | 8        | 0.9           |
| (1,1898) | 1:91:A:VAL:HG12  | 1:92:A:THR:HG22 | 8        | 0.9           |
| (1,1898) | 1:91:A:VAL:HG12  | 1:92:A:THR:HG23 | 8        | 0.9           |
| (1,1898) | 1:91:A:VAL:HG13  | 1:92:A:THR:HG21 | 8        | 0.9           |
| (1,1898) | 1:91:A:VAL:HG13  | 1:92:A:THR:HG22 | 8        | 0.9           |
| (1,1898) | 1:91:A:VAL:HG13  | 1:92:A:THR:HG23 | 8        | 0.9           |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21 | 15       | 0.9           |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22 | 15       | 0.9           |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23 | 15       | 0.9           |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11 | 17       | 0.9           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12  | 17       | 0.9           |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13  | 17       | 0.9           |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11  | 1        | 0.9           |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12  | 1        | 0.9           |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13  | 1        | 0.9           |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11  | 1        | 0.9           |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12  | 1        | 0.9           |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13  | 1        | 0.9           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG11  | 9        | 0.9           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG12  | 9        | 0.9           |
| (1,808)  | 1:34:A:SER:H     | 1:32:A:VAL:HG13  | 9        | 0.9           |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 7        | 0.9           |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 7        | 0.9           |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 7        | 0.9           |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21   | 15       | 0.9           |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22   | 15       | 0.9           |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23   | 15       | 0.9           |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 2        | 0.9           |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 2        | 0.9           |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 2        | 0.9           |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ     | 6        | 0.9           |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ     | 6        | 0.9           |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ     | 6        | 0.9           |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 3        | 0.89          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 3        | 0.89          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 3        | 0.89          |
| (1,2908) | 1:32:A:VAL:HG11  | 1:19:A:GLU:H     | 6        | 0.89          |
| (1,2908) | 1:32:A:VAL:HG12  | 1:19:A:GLU:H     | 6        | 0.89          |
| (1,2908) | 1:32:A:VAL:HG13  | 1:19:A:GLU:H     | 6        | 0.89          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 16       | 0.89          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 16       | 0.89          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 16       | 0.89          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 16       | 0.89          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 16       | 0.89          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 16       | 0.89          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 13       | 0.89          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 13       | 0.89          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 13       | 0.89          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 8        | 0.89          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 8        | 0.89          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 8        | 0.89          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 8        | 0.89          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 8        | 0.89          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 8        | 0.89          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11  | 16       | 0.89          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12  | 16       | 0.89          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13  | 16       | 0.89          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11  | 16       | 0.89          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12  | 16       | 0.89          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13  | 16       | 0.89          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 8        | 0.89          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 8        | 0.89          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 8        | 0.89          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21   | 3        | 0.89          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22   | 3        | 0.89          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23   | 3        | 0.89          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2   | 7        | 0.89          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3   | 7        | 0.89          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2   | 7        | 0.89          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3   | 7        | 0.89          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2   | 7        | 0.89          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3   | 7        | 0.89          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 19       | 0.88          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 19       | 0.88          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 19       | 0.88          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 19       | 0.88          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 19       | 0.88          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 19       | 0.88          |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG11 | 20       | 0.88          |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG12 | 20       | 0.88          |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG13 | 20       | 0.88          |
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG11 | 20       | 0.88          |
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG12 | 20       | 0.88          |
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG13 | 20       | 0.88          |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB2  | 17       | 0.88          |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB3  | 17       | 0.88          |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB2  | 17       | 0.88          |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB3  | 17       | 0.88          |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB2  | 17       | 0.88          |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB3  | 17       | 0.88          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 14       | 0.88          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 14       | 0.88          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 14       | 0.88          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 14       | 0.88          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22  | 14       | 0.88          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23  | 14       | 0.88          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21  | 14       | 0.88          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22  | 14       | 0.88          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23  | 14       | 0.88          |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA    | 20       | 0.88          |
| (1,1776) | 1:37:A:LEU:HD12  | 1:86:A:LEU:HA    | 20       | 0.88          |
| (1,1776) | 1:37:A:LEU:HD13  | 1:86:A:LEU:HA    | 20       | 0.88          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD11  | 20       | 0.88          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12  | 20       | 0.88          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13  | 20       | 0.88          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2   | 12       | 0.88          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3   | 12       | 0.88          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2   | 12       | 0.88          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3   | 12       | 0.88          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2   | 12       | 0.88          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3   | 12       | 0.88          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21   | 14       | 0.88          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22   | 14       | 0.88          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23   | 14       | 0.88          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21   | 14       | 0.88          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22   | 14       | 0.88          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23   | 14       | 0.88          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 16       | 0.87          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 16       | 0.87          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 16       | 0.87          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 6        | 0.87          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 6        | 0.87          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 6        | 0.87          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 6        | 0.87          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 6        | 0.87          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 6        | 0.87          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 14       | 0.87          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 14       | 0.87          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 14       | 0.87          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 14       | 0.87          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 14       | 0.87          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 14       | 0.87          |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG11 | 1        | 0.87          |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG12 | 1        | 0.87          |
| (1,2417) | 1:21:A:PHE:HD1   | 1:119:A:VAL:HG13 | 1        | 0.87          |
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG11 | 1        | 0.87          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG12 | 1        | 0.87          |
| (1,2417) | 1:21:A:PHE:HD2   | 1:119:A:VAL:HG13 | 1        | 0.87          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 9        | 0.87          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 9        | 0.87          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 9        | 0.87          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 9        | 0.87          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 9        | 0.87          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 9        | 0.87          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 2        | 0.87          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 2        | 0.87          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 2        | 0.87          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 2        | 0.87          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 2        | 0.87          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 2        | 0.87          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 2        | 0.87          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 2        | 0.87          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 2        | 0.87          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 2        | 0.87          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 2        | 0.87          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 2        | 0.87          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11  | 12       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12  | 12       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13  | 12       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11  | 12       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12  | 12       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13  | 12       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11  | 15       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12  | 15       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13  | 15       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11  | 15       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12  | 15       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13  | 15       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11  | 19       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12  | 19       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13  | 19       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11  | 19       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12  | 19       | 0.87          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13  | 19       | 0.87          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 18       | 0.87          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 18       | 0.87          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 18       | 0.87          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11  | 19       | 0.87          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,807)  | 1:6:A:PHE:H     | 1:32:A:VAL:HG12 | 19       | 0.87          |
| (1,807)  | 1:6:A:PHE:H     | 1:32:A:VAL:HG13 | 19       | 0.87          |
| (1,516)  | 1:32:A:VAL:HG11 | 1:19:A:GLU:HB2  | 15       | 0.87          |
| (1,516)  | 1:32:A:VAL:HG11 | 1:19:A:GLU:HB3  | 15       | 0.87          |
| (1,516)  | 1:32:A:VAL:HG12 | 1:19:A:GLU:HB2  | 15       | 0.87          |
| (1,516)  | 1:32:A:VAL:HG12 | 1:19:A:GLU:HB3  | 15       | 0.87          |
| (1,516)  | 1:32:A:VAL:HG13 | 1:19:A:GLU:HB2  | 15       | 0.87          |
| (1,516)  | 1:32:A:VAL:HG13 | 1:19:A:GLU:HB3  | 15       | 0.87          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG21  | 16       | 0.87          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG22  | 16       | 0.87          |
| (1,276)  | 1:77:A:ILE:H    | 1:4:A:VAL:HG23  | 16       | 0.87          |
| (1,272)  | 1:6:A:PHE:HD1   | 1:4:A:VAL:HG21  | 8        | 0.87          |
| (1,272)  | 1:6:A:PHE:HD1   | 1:4:A:VAL:HG22  | 8        | 0.87          |
| (1,272)  | 1:6:A:PHE:HD1   | 1:4:A:VAL:HG23  | 8        | 0.87          |
| (1,272)  | 1:6:A:PHE:HD2   | 1:4:A:VAL:HG21  | 8        | 0.87          |
| (1,272)  | 1:6:A:PHE:HD2   | 1:4:A:VAL:HG22  | 8        | 0.87          |
| (1,272)  | 1:6:A:PHE:HD2   | 1:4:A:VAL:HG23  | 8        | 0.87          |
| (1,49)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG2  | 3        | 0.87          |
| (1,49)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG3  | 3        | 0.87          |
| (1,49)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG2  | 3        | 0.87          |
| (1,49)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG3  | 3        | 0.87          |
| (1,49)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG2  | 3        | 0.87          |
| (1,49)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG3  | 3        | 0.87          |
| (1,47)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG2  | 3        | 0.87          |
| (1,47)   | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG3  | 3        | 0.87          |
| (1,47)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG2  | 3        | 0.87          |
| (1,47)   | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG3  | 3        | 0.87          |
| (1,47)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG2  | 3        | 0.87          |
| (1,47)   | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG3  | 3        | 0.87          |
| (1,3349) | 1:4:A:VAL:HG21  | 1:77:A:ILE:H    | 9        | 0.86          |
| (1,3349) | 1:4:A:VAL:HG22  | 1:77:A:ILE:H    | 9        | 0.86          |
| (1,3349) | 1:4:A:VAL:HG23  | 1:77:A:ILE:H    | 9        | 0.86          |
| (1,2781) | 1:35:A:SER:H    | 1:79:A:LEU:HD11 | 15       | 0.86          |
| (1,2781) | 1:35:A:SER:H    | 1:79:A:LEU:HD12 | 15       | 0.86          |
| (1,2781) | 1:35:A:SER:H    | 1:79:A:LEU:HD13 | 15       | 0.86          |
| (1,845)  | 1:79:A:LEU:HD11 | 1:34:A:SER:HA   | 10       | 0.86          |
| (1,845)  | 1:79:A:LEU:HD12 | 1:34:A:SER:HA   | 10       | 0.86          |
| (1,845)  | 1:79:A:LEU:HD13 | 1:34:A:SER:HA   | 10       | 0.86          |
| (1,516)  | 1:32:A:VAL:HG11 | 1:19:A:GLU:HB2  | 7        | 0.86          |
| (1,516)  | 1:32:A:VAL:HG11 | 1:19:A:GLU:HB3  | 7        | 0.86          |
| (1,516)  | 1:32:A:VAL:HG12 | 1:19:A:GLU:HB2  | 7        | 0.86          |
| (1,516)  | 1:32:A:VAL:HG12 | 1:19:A:GLU:HB3  | 7        | 0.86          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2  | 7        | 0.86          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3  | 7        | 0.86          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2  | 8        | 0.86          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3  | 8        | 0.86          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2  | 8        | 0.86          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3  | 8        | 0.86          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2  | 8        | 0.86          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3  | 8        | 0.86          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21  | 1        | 0.86          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22  | 1        | 0.86          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23  | 1        | 0.86          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21  | 9        | 0.86          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22  | 9        | 0.86          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23  | 9        | 0.86          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ    | 10       | 0.86          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ    | 10       | 0.86          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ    | 10       | 0.86          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H    | 3        | 0.86          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H    | 3        | 0.86          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H    | 3        | 0.86          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H    | 17       | 0.86          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H    | 17       | 0.86          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H    | 17       | 0.86          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H    | 20       | 0.86          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H    | 20       | 0.86          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H    | 20       | 0.86          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H   | 9        | 0.85          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H   | 9        | 0.85          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H   | 9        | 0.85          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2 | 8        | 0.85          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3 | 8        | 0.85          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2 | 8        | 0.85          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3 | 8        | 0.85          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2 | 8        | 0.85          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3 | 8        | 0.85          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA  | 15       | 0.85          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA  | 15       | 0.85          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA  | 15       | 0.85          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11 | 12       | 0.85          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12 | 12       | 0.85          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13 | 12       | 0.85          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21  | 3        | 0.85          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 3        | 0.85          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 3        | 0.85          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 20       | 0.85          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 20       | 0.85          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 20       | 0.85          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21   | 20       | 0.85          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22   | 20       | 0.85          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23   | 20       | 0.85          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21   | 20       | 0.85          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22   | 20       | 0.85          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23   | 20       | 0.85          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 4        | 0.85          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 4        | 0.85          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 4        | 0.85          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 4        | 0.85          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 4        | 0.85          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 4        | 0.85          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 4        | 0.85          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 4        | 0.85          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 4        | 0.85          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 4        | 0.85          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 4        | 0.85          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 4        | 0.85          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 2        | 0.84          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 2        | 0.84          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 2        | 0.84          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 4        | 0.84          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 4        | 0.84          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 4        | 0.84          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 11       | 0.84          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 11       | 0.84          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 11       | 0.84          |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG21 | 19       | 0.84          |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG22 | 19       | 0.84          |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG23 | 19       | 0.84          |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG21 | 19       | 0.84          |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG22 | 19       | 0.84          |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG23 | 19       | 0.84          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 4        | 0.84          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 4        | 0.84          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 4        | 0.84          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 4        | 0.84          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22 | 4        | 0.84          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23 | 4        | 0.84          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21 | 4        | 0.84          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22 | 4        | 0.84          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23 | 4        | 0.84          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21 | 10       | 0.84          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22 | 10       | 0.84          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23 | 10       | 0.84          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21 | 10       | 0.84          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22 | 10       | 0.84          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23 | 10       | 0.84          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21 | 10       | 0.84          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22 | 10       | 0.84          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23 | 10       | 0.84          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21 | 6        | 0.84          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22 | 6        | 0.84          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23 | 6        | 0.84          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11 | 4        | 0.84          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12 | 4        | 0.84          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13 | 4        | 0.84          |
| (1,1684) | 1:4:A:VAL:HG21   | 1:77:A:ILE:HG12 | 4        | 0.84          |
| (1,1684) | 1:4:A:VAL:HG21   | 1:77:A:ILE:HG13 | 4        | 0.84          |
| (1,1684) | 1:4:A:VAL:HG22   | 1:77:A:ILE:HG12 | 4        | 0.84          |
| (1,1684) | 1:4:A:VAL:HG22   | 1:77:A:ILE:HG13 | 4        | 0.84          |
| (1,1684) | 1:4:A:VAL:HG23   | 1:77:A:ILE:HG12 | 4        | 0.84          |
| (1,1684) | 1:4:A:VAL:HG23   | 1:77:A:ILE:HG13 | 4        | 0.84          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11 | 17       | 0.84          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12 | 17       | 0.84          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13 | 17       | 0.84          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11 | 17       | 0.84          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12 | 17       | 0.84          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13 | 17       | 0.84          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG11 | 7        | 0.84          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG12 | 7        | 0.84          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG13 | 7        | 0.84          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG11 | 7        | 0.84          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG12 | 7        | 0.84          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG13 | 7        | 0.84          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21  | 2        | 0.84          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22  | 2        | 0.84          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23  | 2        | 0.84          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21  | 4        | 0.84          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22  | 4        | 0.84          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23  | 4        | 0.84          |
| (1,142)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE1   | 16       | 0.84          |
| (1,142)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE2   | 16       | 0.84          |
| (1,142)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE1   | 16       | 0.84          |
| (1,142)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE2   | 16       | 0.84          |
| (1,142)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE1   | 16       | 0.84          |
| (1,142)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE2   | 16       | 0.84          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1   | 17       | 0.84          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2   | 17       | 0.84          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1   | 17       | 0.84          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2   | 17       | 0.84          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1   | 17       | 0.84          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2   | 17       | 0.84          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H    | 8        | 0.83          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H    | 8        | 0.83          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H    | 8        | 0.83          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21 | 9        | 0.83          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22 | 9        | 0.83          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23 | 9        | 0.83          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21 | 9        | 0.83          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22 | 9        | 0.83          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23 | 9        | 0.83          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21 | 9        | 0.83          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22 | 9        | 0.83          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23 | 9        | 0.83          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11 | 5        | 0.83          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12 | 5        | 0.83          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13 | 5        | 0.83          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11 | 5        | 0.83          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12 | 5        | 0.83          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13 | 5        | 0.83          |
| (1,1233) | 1:53:A:VAL:HG11  | 1:52:A:GLU:HG2  | 3        | 0.83          |
| (1,1233) | 1:53:A:VAL:HG11  | 1:52:A:GLU:HG3  | 3        | 0.83          |
| (1,1233) | 1:53:A:VAL:HG12  | 1:52:A:GLU:HG2  | 3        | 0.83          |
| (1,1233) | 1:53:A:VAL:HG12  | 1:52:A:GLU:HG3  | 3        | 0.83          |
| (1,1233) | 1:53:A:VAL:HG13  | 1:52:A:GLU:HG2  | 3        | 0.83          |
| (1,1233) | 1:53:A:VAL:HG13  | 1:52:A:GLU:HG3  | 3        | 0.83          |
| (1,1233) | 1:53:A:VAL:HG11  | 1:52:A:GLU:HG2  | 3        | 0.83          |
| (1,1233) | 1:53:A:VAL:HG11  | 1:52:A:GLU:HG3  | 3        | 0.83          |
| (1,1233) | 1:53:A:VAL:HG12  | 1:52:A:GLU:HG2  | 3        | 0.83          |
| (1,1233) | 1:53:A:VAL:HG12  | 1:52:A:GLU:HG3  | 3        | 0.83          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1233) | 1:53:A:VAL:HG13  | 1:52:A:GLU:HG2  | 3        | 0.83          |
| (1,1233) | 1:53:A:VAL:HG13  | 1:52:A:GLU:HG3  | 3        | 0.83          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 20       | 0.83          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 20       | 0.83          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 20       | 0.83          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21  | 8        | 0.83          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22  | 8        | 0.83          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23  | 8        | 0.83          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21  | 11       | 0.83          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22  | 11       | 0.83          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23  | 11       | 0.83          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21  | 11       | 0.83          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22  | 11       | 0.83          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23  | 11       | 0.83          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB    | 9        | 0.83          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB    | 9        | 0.83          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB    | 9        | 0.83          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB    | 14       | 0.83          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB    | 14       | 0.83          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB    | 14       | 0.83          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H   | 11       | 0.82          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H   | 11       | 0.82          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H   | 11       | 0.82          |
| (1,2084) | 1:79:A:LEU:HD21  | 1:101:A:LEU:HG  | 8        | 0.82          |
| (1,2084) | 1:79:A:LEU:HD22  | 1:101:A:LEU:HG  | 8        | 0.82          |
| (1,2084) | 1:79:A:LEU:HD23  | 1:101:A:LEU:HG  | 8        | 0.82          |
| (1,845)  | 1:79:A:LEU:HD11  | 1:34:A:SER:HA   | 15       | 0.82          |
| (1,845)  | 1:79:A:LEU:HD12  | 1:34:A:SER:HA   | 15       | 0.82          |
| (1,845)  | 1:79:A:LEU:HD13  | 1:34:A:SER:HA   | 15       | 0.82          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21 | 17       | 0.82          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22 | 17       | 0.82          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23 | 17       | 0.82          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21 | 17       | 0.82          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22 | 17       | 0.82          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23 | 17       | 0.82          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21 | 17       | 0.82          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22 | 17       | 0.82          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23 | 17       | 0.82          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11 | 13       | 0.82          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12 | 13       | 0.82          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13 | 13       | 0.82          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11 | 13       | 0.82          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12  | 13       | 0.82          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13  | 13       | 0.82          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 4        | 0.82          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 4        | 0.82          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 4        | 0.82          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 11       | 0.82          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 11       | 0.82          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 11       | 0.82          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 13       | 0.82          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 13       | 0.82          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 13       | 0.82          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 13       | 0.82          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 13       | 0.82          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 13       | 0.82          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H     | 19       | 0.82          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H     | 19       | 0.82          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H     | 19       | 0.82          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 18       | 0.82          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 18       | 0.82          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 18       | 0.82          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 18       | 0.82          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 18       | 0.82          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 18       | 0.82          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 18       | 0.82          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 18       | 0.82          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 18       | 0.82          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 18       | 0.82          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 18       | 0.82          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 18       | 0.82          |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG21 | 20       | 0.81          |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG22 | 20       | 0.81          |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG23 | 20       | 0.81          |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG21 | 20       | 0.81          |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG22 | 20       | 0.81          |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG23 | 20       | 0.81          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 12       | 0.81          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 12       | 0.81          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 12       | 0.81          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 12       | 0.81          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22  | 12       | 0.81          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23  | 12       | 0.81          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21  | 12       | 0.81          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22  | 12       | 0.81          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23  | 12       | 0.81          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 11       | 0.81          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 11       | 0.81          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 11       | 0.81          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 19       | 0.81          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 19       | 0.81          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 19       | 0.81          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21   | 4        | 0.81          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22   | 4        | 0.81          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23   | 4        | 0.81          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21   | 4        | 0.81          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22   | 4        | 0.81          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23   | 4        | 0.81          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 12       | 0.81          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 12       | 0.81          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 12       | 0.81          |
| (1,144)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HZ     | 13       | 0.81          |
| (1,144)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HZ     | 13       | 0.81          |
| (1,144)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HZ     | 13       | 0.81          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 3        | 0.8           |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 3        | 0.8           |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 3        | 0.8           |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 3        | 0.8           |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 3        | 0.8           |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 3        | 0.8           |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG21 | 1        | 0.8           |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG22 | 1        | 0.8           |
| (1,2427) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HG23 | 1        | 0.8           |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG21 | 1        | 0.8           |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG22 | 1        | 0.8           |
| (1,2427) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HG23 | 1        | 0.8           |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 7        | 0.8           |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 7        | 0.8           |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 7        | 0.8           |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 7        | 0.8           |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22  | 7        | 0.8           |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23  | 7        | 0.8           |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21  | 7        | 0.8           |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22  | 7        | 0.8           |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23  | 7        | 0.8           |
| (1,1737) | 1:15:A:SER:HB2   | 1:79:A:LEU:HD11  | 16       | 0.8           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1737) | 1:15:A:SER:HB2   | 1:79:A:LEU:HD12 | 16       | 0.8           |
| (1,1737) | 1:15:A:SER:HB2   | 1:79:A:LEU:HD13 | 16       | 0.8           |
| (1,1737) | 1:15:A:SER:HB3   | 1:79:A:LEU:HD11 | 16       | 0.8           |
| (1,1737) | 1:15:A:SER:HB3   | 1:79:A:LEU:HD12 | 16       | 0.8           |
| (1,1737) | 1:15:A:SER:HB3   | 1:79:A:LEU:HD13 | 16       | 0.8           |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 7        | 0.8           |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 7        | 0.8           |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 7        | 0.8           |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H    | 2        | 0.8           |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H    | 2        | 0.8           |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H    | 2        | 0.8           |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2 | 10       | 0.79          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3 | 10       | 0.79          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2 | 10       | 0.79          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3 | 10       | 0.79          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2 | 10       | 0.79          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3 | 10       | 0.79          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 6        | 0.79          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 6        | 0.79          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 6        | 0.79          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 6        | 0.79          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 6        | 0.79          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 6        | 0.79          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 6        | 0.79          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 6        | 0.79          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 6        | 0.79          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 6        | 0.79          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 6        | 0.79          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 6        | 0.79          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21 | 5        | 0.79          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22 | 5        | 0.79          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23 | 5        | 0.79          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21 | 5        | 0.79          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22 | 5        | 0.79          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23 | 5        | 0.79          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21 | 5        | 0.79          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22 | 5        | 0.79          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23 | 5        | 0.79          |
| (1,1755) | 1:91:A:VAL:HG21  | 1:83:A:GLY:HA2  | 11       | 0.79          |
| (1,1755) | 1:91:A:VAL:HG21  | 1:83:A:GLY:HA3  | 11       | 0.79          |
| (1,1755) | 1:91:A:VAL:HG22  | 1:83:A:GLY:HA2  | 11       | 0.79          |
| (1,1755) | 1:91:A:VAL:HG22  | 1:83:A:GLY:HA3  | 11       | 0.79          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1755) | 1:91:A:VAL:HG23  | 1:83:A:GLY:HA2   | 11       | 0.79          |
| (1,1755) | 1:91:A:VAL:HG23  | 1:83:A:GLY:HA3   | 11       | 0.79          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 6        | 0.79          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 6        | 0.79          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 6        | 0.79          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 11       | 0.79          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 11       | 0.79          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 11       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21   | 15       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22   | 15       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23   | 15       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21   | 15       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22   | 15       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23   | 15       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21   | 19       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22   | 19       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23   | 19       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21   | 19       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22   | 19       | 0.79          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23   | 19       | 0.79          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 18       | 0.78          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 18       | 0.78          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 18       | 0.78          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 14       | 0.78          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 14       | 0.78          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 14       | 0.78          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 14       | 0.78          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 14       | 0.78          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 14       | 0.78          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 11       | 0.78          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 11       | 0.78          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 11       | 0.78          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 11       | 0.78          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 11       | 0.78          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 11       | 0.78          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 11       | 0.78          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 11       | 0.78          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 11       | 0.78          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 11       | 0.78          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 11       | 0.78          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 11       | 0.78          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD11  | 18       | 0.78          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,910) | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD12 | 18       | 0.78          |
| (1,910) | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD13 | 18       | 0.78          |
| (1,910) | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD11 | 18       | 0.78          |
| (1,910) | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD12 | 18       | 0.78          |
| (1,910) | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD13 | 18       | 0.78          |
| (1,910) | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD11 | 18       | 0.78          |
| (1,910) | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD12 | 18       | 0.78          |
| (1,910) | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD13 | 18       | 0.78          |
| (1,516) | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2  | 18       | 0.78          |
| (1,516) | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3  | 18       | 0.78          |
| (1,516) | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2  | 18       | 0.78          |
| (1,516) | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3  | 18       | 0.78          |
| (1,516) | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2  | 18       | 0.78          |
| (1,516) | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3  | 18       | 0.78          |
| (1,323) | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21  | 2        | 0.78          |
| (1,323) | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22  | 2        | 0.78          |
| (1,323) | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23  | 2        | 0.78          |
| (1,276) | 1:77:A:ILE:H     | 1:4:A:VAL:HG21  | 18       | 0.78          |
| (1,276) | 1:77:A:ILE:H     | 1:4:A:VAL:HG22  | 18       | 0.78          |
| (1,276) | 1:77:A:ILE:H     | 1:4:A:VAL:HG23  | 18       | 0.78          |
| (1,142) | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE1   | 7        | 0.78          |
| (1,142) | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE2   | 7        | 0.78          |
| (1,142) | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE1   | 7        | 0.78          |
| (1,142) | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE2   | 7        | 0.78          |
| (1,142) | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE1   | 7        | 0.78          |
| (1,142) | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE2   | 7        | 0.78          |
| (1,142) | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE1   | 9        | 0.78          |
| (1,142) | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE2   | 9        | 0.78          |
| (1,142) | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE1   | 9        | 0.78          |
| (1,142) | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE2   | 9        | 0.78          |
| (1,142) | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE1   | 9        | 0.78          |
| (1,142) | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE2   | 9        | 0.78          |
| (1,49)  | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2  | 14       | 0.78          |
| (1,49)  | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3  | 14       | 0.78          |
| (1,49)  | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2  | 14       | 0.78          |
| (1,49)  | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3  | 14       | 0.78          |
| (1,49)  | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2  | 14       | 0.78          |
| (1,49)  | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3  | 14       | 0.78          |
| (1,47)  | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2  | 14       | 0.78          |
| (1,47)  | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3  | 14       | 0.78          |
| (1,47)  | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2  | 14       | 0.78          |
| (1,47)  | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3  | 14       | 0.78          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 14       | 0.78          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 14       | 0.78          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H    | 8        | 0.77          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H    | 8        | 0.77          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H    | 8        | 0.77          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 9        | 0.77          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 9        | 0.77          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 9        | 0.77          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 9        | 0.77          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 9        | 0.77          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 9        | 0.77          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 18       | 0.77          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 18       | 0.77          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 18       | 0.77          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 18       | 0.77          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22  | 18       | 0.77          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23  | 18       | 0.77          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21  | 18       | 0.77          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22  | 18       | 0.77          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23  | 18       | 0.77          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11  | 3        | 0.77          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12  | 3        | 0.77          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13  | 3        | 0.77          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H    | 17       | 0.76          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H    | 17       | 0.76          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H    | 17       | 0.76          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 18       | 0.76          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 18       | 0.76          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 18       | 0.76          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 18       | 0.76          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 18       | 0.76          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 18       | 0.76          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 14       | 0.76          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 14       | 0.76          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 14       | 0.76          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 14       | 0.76          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 14       | 0.76          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 14       | 0.76          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 18       | 0.76          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 18       | 0.76          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 18       | 0.76          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 18       | 0.76          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 18       | 0.76          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 18       | 0.76          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 10       | 0.76          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 10       | 0.76          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 10       | 0.76          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 16       | 0.76          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 16       | 0.76          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 16       | 0.76          |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 20       | 0.76          |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 20       | 0.76          |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 20       | 0.76          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ     | 16       | 0.76          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ     | 16       | 0.76          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ     | 16       | 0.76          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H     | 14       | 0.76          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H     | 14       | 0.76          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H     | 14       | 0.76          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H    | 19       | 0.75          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H    | 19       | 0.75          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H    | 19       | 0.75          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG11 | 4        | 0.75          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG12 | 4        | 0.75          |
| (1,2561) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HG13 | 4        | 0.75          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG11 | 4        | 0.75          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG12 | 4        | 0.75          |
| (1,2561) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HG13 | 4        | 0.75          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 10       | 0.75          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 10       | 0.75          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 10       | 0.75          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 10       | 0.75          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 10       | 0.75          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 10       | 0.75          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 10       | 0.75          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 10       | 0.75          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 10       | 0.75          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 10       | 0.75          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 10       | 0.75          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 10       | 0.75          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 1        | 0.75          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 1        | 0.75          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 1        | 0.75          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 1        | 0.75          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22 | 1        | 0.75          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23 | 1        | 0.75          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21 | 1        | 0.75          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22 | 1        | 0.75          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23 | 1        | 0.75          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11 | 8        | 0.75          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12 | 8        | 0.75          |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13 | 8        | 0.75          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11 | 8        | 0.75          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12 | 8        | 0.75          |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13 | 8        | 0.75          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11 | 5        | 0.75          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12 | 5        | 0.75          |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13 | 5        | 0.75          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD11 | 16       | 0.75          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD12 | 16       | 0.75          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD13 | 16       | 0.75          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD11 | 16       | 0.75          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD12 | 16       | 0.75          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD13 | 16       | 0.75          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD11 | 16       | 0.75          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD12 | 16       | 0.75          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD13 | 16       | 0.75          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21 | 9        | 0.75          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22 | 9        | 0.75          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23 | 9        | 0.75          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21 | 9        | 0.75          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22 | 9        | 0.75          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23 | 9        | 0.75          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21 | 9        | 0.75          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22 | 9        | 0.75          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23 | 9        | 0.75          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21  | 12       | 0.75          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22  | 12       | 0.75          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23  | 12       | 0.75          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21  | 2        | 0.75          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22  | 2        | 0.75          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23  | 2        | 0.75          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21  | 2        | 0.75          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22  | 2        | 0.75          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23  | 2        | 0.75          |
| (1,2746) | 1:119:A:VAL:HG21 | 1:15:A:SER:HA   | 19       | 0.74          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2746) | 1:119:A:VAL:HG22 | 1:15:A:SER:HA   | 19       | 0.74          |
| (1,2746) | 1:119:A:VAL:HG23 | 1:15:A:SER:HA   | 19       | 0.74          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA  | 9        | 0.74          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA  | 9        | 0.74          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA  | 9        | 0.74          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21 | 8        | 0.74          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22 | 8        | 0.74          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23 | 8        | 0.74          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21 | 8        | 0.74          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22 | 8        | 0.74          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23 | 8        | 0.74          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21 | 8        | 0.74          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22 | 8        | 0.74          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23 | 8        | 0.74          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21 | 20       | 0.74          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22 | 20       | 0.74          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23 | 20       | 0.74          |
| (1,1684) | 1:4:A:VAL:HG21   | 1:77:A:ILE:HG12 | 6        | 0.74          |
| (1,1684) | 1:4:A:VAL:HG21   | 1:77:A:ILE:HG13 | 6        | 0.74          |
| (1,1684) | 1:4:A:VAL:HG22   | 1:77:A:ILE:HG12 | 6        | 0.74          |
| (1,1684) | 1:4:A:VAL:HG22   | 1:77:A:ILE:HG13 | 6        | 0.74          |
| (1,1684) | 1:4:A:VAL:HG23   | 1:77:A:ILE:HG12 | 6        | 0.74          |
| (1,1684) | 1:4:A:VAL:HG23   | 1:77:A:ILE:HG13 | 6        | 0.74          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21 | 18       | 0.74          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG22 | 18       | 0.74          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG23 | 18       | 0.74          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 14       | 0.74          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 14       | 0.74          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 14       | 0.74          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2  | 6        | 0.74          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3  | 6        | 0.74          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2  | 6        | 0.74          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3  | 6        | 0.74          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2  | 6        | 0.74          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3  | 6        | 0.74          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11  | 9        | 0.74          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12  | 9        | 0.74          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13  | 9        | 0.74          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11  | 9        | 0.74          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12  | 9        | 0.74          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13  | 9        | 0.74          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21  | 5        | 0.74          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22  | 5        | 0.74          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23  | 5        | 0.74          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21  | 5        | 0.74          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22  | 5        | 0.74          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23  | 5        | 0.74          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21  | 18       | 0.74          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22  | 18       | 0.74          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23  | 18       | 0.74          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21  | 18       | 0.74          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22  | 18       | 0.74          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23  | 18       | 0.74          |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG11  | 13       | 0.74          |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG12  | 13       | 0.74          |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG13  | 13       | 0.74          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H   | 2        | 0.73          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H   | 2        | 0.73          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H   | 2        | 0.73          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 7        | 0.73          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 7        | 0.73          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 7        | 0.73          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 7        | 0.73          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 7        | 0.73          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 7        | 0.73          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 7        | 0.73          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 7        | 0.73          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 7        | 0.73          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 7        | 0.73          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 7        | 0.73          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 7        | 0.73          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21  | 18       | 0.73          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22  | 18       | 0.73          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23  | 18       | 0.73          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21  | 1        | 0.73          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22  | 1        | 0.73          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23  | 1        | 0.73          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21  | 1        | 0.73          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22  | 1        | 0.73          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23  | 1        | 0.73          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21  | 16       | 0.73          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22  | 16       | 0.73          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23  | 16       | 0.73          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21  | 16       | 0.73          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22  | 16       | 0.73          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23  | 16       | 0.73          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H   | 5        | 0.72          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H   | 5        | 0.72          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H   | 5        | 0.72          |
| (1,1664) | 1:79:A:LEU:HD21  | 1:77:A:ILE:HA   | 15       | 0.72          |
| (1,1664) | 1:79:A:LEU:HD22  | 1:77:A:ILE:HA   | 15       | 0.72          |
| (1,1664) | 1:79:A:LEU:HD23  | 1:77:A:ILE:HA   | 15       | 0.72          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11 | 20       | 0.72          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12 | 20       | 0.72          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13 | 20       | 0.72          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11 | 20       | 0.72          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12 | 20       | 0.72          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13 | 20       | 0.72          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21 | 16       | 0.72          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22 | 16       | 0.72          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23 | 16       | 0.72          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21 | 16       | 0.72          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22 | 16       | 0.72          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23 | 16       | 0.72          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21 | 16       | 0.72          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22 | 16       | 0.72          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23 | 16       | 0.72          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11 | 19       | 0.72          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12 | 19       | 0.72          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13 | 19       | 0.72          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11 | 19       | 0.72          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12 | 19       | 0.72          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13 | 19       | 0.72          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG11 | 13       | 0.72          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG12 | 13       | 0.72          |
| (1,799)  | 1:23:A:LYS:HG2   | 1:32:A:VAL:HG13 | 13       | 0.72          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG11 | 13       | 0.72          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG12 | 13       | 0.72          |
| (1,799)  | 1:23:A:LYS:HG3   | 1:32:A:VAL:HG13 | 13       | 0.72          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1   | 19       | 0.72          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2   | 19       | 0.72          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1   | 19       | 0.72          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2   | 19       | 0.72          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1   | 19       | 0.72          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2   | 19       | 0.72          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H   | 7        | 0.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H    | 7        | 0.71          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H    | 7        | 0.71          |
| (1,2744) | 1:79:A:LEU:HD11  | 1:15:A:SER:HA    | 10       | 0.71          |
| (1,2744) | 1:79:A:LEU:HD12  | 1:15:A:SER:HA    | 10       | 0.71          |
| (1,2744) | 1:79:A:LEU:HD13  | 1:15:A:SER:HA    | 10       | 0.71          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD11  | 10       | 0.71          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD12  | 10       | 0.71          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD13  | 10       | 0.71          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD21  | 9        | 0.71          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD22  | 9        | 0.71          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD23  | 9        | 0.71          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD21  | 9        | 0.71          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD22  | 9        | 0.71          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD23  | 9        | 0.71          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21   | 12       | 0.71          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22   | 12       | 0.71          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23   | 12       | 0.71          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21   | 12       | 0.71          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22   | 12       | 0.71          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23   | 12       | 0.71          |
| (1,144)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HZ     | 10       | 0.71          |
| (1,144)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HZ     | 10       | 0.71          |
| (1,144)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HZ     | 10       | 0.71          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 3        | 0.7           |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 3        | 0.7           |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 3        | 0.7           |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 3        | 0.7           |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 3        | 0.7           |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 3        | 0.7           |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 7        | 0.7           |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 7        | 0.7           |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 7        | 0.7           |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 12       | 0.7           |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 12       | 0.7           |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 12       | 0.7           |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 12       | 0.7           |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 12       | 0.7           |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 12       | 0.7           |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 9        | 0.7           |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 9        | 0.7           |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 9        | 0.7           |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG11  | 18       | 0.7           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG12  | 18       | 0.7           |
| (1,1244) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG13  | 18       | 0.7           |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG11  | 18       | 0.7           |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG12  | 18       | 0.7           |
| (1,1244) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG13  | 18       | 0.7           |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD11  | 5        | 0.7           |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD12  | 5        | 0.7           |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD13  | 5        | 0.7           |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD11  | 5        | 0.7           |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD12  | 5        | 0.7           |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD13  | 5        | 0.7           |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD11  | 5        | 0.7           |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD12  | 5        | 0.7           |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD13  | 5        | 0.7           |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21   | 10       | 0.7           |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22   | 10       | 0.7           |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23   | 10       | 0.7           |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21   | 10       | 0.7           |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22   | 10       | 0.7           |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23   | 10       | 0.7           |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG11   | 7        | 0.7           |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG12   | 7        | 0.7           |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG13   | 7        | 0.7           |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ     | 17       | 0.7           |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ     | 17       | 0.7           |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ     | 17       | 0.7           |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA    | 14       | 0.7           |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA    | 14       | 0.7           |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA    | 14       | 0.7           |
| (1,2744) | 1:79:A:LEU:HD11  | 1:15:A:SER:HA    | 8        | 0.69          |
| (1,2744) | 1:79:A:LEU:HD12  | 1:15:A:SER:HA    | 8        | 0.69          |
| (1,2744) | 1:79:A:LEU:HD13  | 1:15:A:SER:HA    | 8        | 0.69          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 20       | 0.69          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 20       | 0.69          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 20       | 0.69          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 14       | 0.69          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 14       | 0.69          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 14       | 0.69          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 14       | 0.69          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 14       | 0.69          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 14       | 0.69          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 14       | 0.69          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 14       | 0.69          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 14       | 0.69          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 14       | 0.69          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 14       | 0.69          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 14       | 0.69          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD11 | 8        | 0.69          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD12 | 8        | 0.69          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD13 | 8        | 0.69          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11 | 8        | 0.69          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12 | 8        | 0.69          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13 | 8        | 0.69          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11 | 8        | 0.69          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12 | 8        | 0.69          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13 | 8        | 0.69          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 12       | 0.69          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 12       | 0.69          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 12       | 0.69          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA   | 20       | 0.69          |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA   | 20       | 0.69          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA   | 20       | 0.69          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11  | 11       | 0.69          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12  | 11       | 0.69          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13  | 11       | 0.69          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11  | 11       | 0.69          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12  | 11       | 0.69          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13  | 11       | 0.69          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ    | 12       | 0.69          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ    | 12       | 0.69          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ    | 12       | 0.69          |
| (1,142)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE1   | 13       | 0.69          |
| (1,142)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE2   | 13       | 0.69          |
| (1,142)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE1   | 13       | 0.69          |
| (1,142)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE2   | 13       | 0.69          |
| (1,142)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE1   | 13       | 0.69          |
| (1,142)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE2   | 13       | 0.69          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H    | 4        | 0.69          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H    | 4        | 0.69          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H    | 4        | 0.69          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA   | 3        | 0.69          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA   | 3        | 0.69          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA   | 3        | 0.69          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA   | 5        | 0.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA    | 5        | 0.69          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA    | 5        | 0.69          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA    | 17       | 0.69          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA    | 17       | 0.69          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA    | 17       | 0.69          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H    | 14       | 0.68          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H    | 14       | 0.68          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H    | 14       | 0.68          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 18       | 0.68          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 18       | 0.68          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 18       | 0.68          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 10       | 0.68          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 10       | 0.68          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 10       | 0.68          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 10       | 0.68          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 10       | 0.68          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 10       | 0.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 10       | 0.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 10       | 0.68          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 10       | 0.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 10       | 0.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 10       | 0.68          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 10       | 0.68          |
| (1,1794) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HG    | 9        | 0.68          |
| (1,1794) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HG    | 9        | 0.68          |
| (1,1794) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HG    | 9        | 0.68          |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA    | 5        | 0.68          |
| (1,1776) | 1:37:A:LEU:HD12  | 1:86:A:LEU:HA    | 5        | 0.68          |
| (1,1776) | 1:37:A:LEU:HD13  | 1:86:A:LEU:HA    | 5        | 0.68          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11  | 1        | 0.68          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12  | 1        | 0.68          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13  | 1        | 0.68          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11  | 1        | 0.68          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12  | 1        | 0.68          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13  | 1        | 0.68          |
| (1,1216) | 1:53:A:VAL:HG21  | 1:52:A:GLU:HA    | 9        | 0.68          |
| (1,1216) | 1:53:A:VAL:HG22  | 1:52:A:GLU:HA    | 9        | 0.68          |
| (1,1216) | 1:53:A:VAL:HG23  | 1:52:A:GLU:HA    | 9        | 0.68          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD11  | 5        | 0.68          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12  | 5        | 0.68          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13  | 5        | 0.68          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG21  | 5        | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG22  | 5        | 0.68          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG23  | 5        | 0.68          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21   | 3        | 0.68          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22   | 3        | 0.68          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23   | 3        | 0.68          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21   | 3        | 0.68          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22   | 3        | 0.68          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23   | 3        | 0.68          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2   | 17       | 0.68          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3   | 17       | 0.68          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2   | 17       | 0.68          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3   | 17       | 0.68          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2   | 17       | 0.68          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3   | 17       | 0.68          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA    | 6        | 0.68          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA    | 6        | 0.68          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA    | 6        | 0.68          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H    | 4        | 0.67          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H    | 4        | 0.67          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H    | 4        | 0.67          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H    | 10       | 0.67          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H    | 10       | 0.67          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H    | 10       | 0.67          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 1        | 0.67          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 1        | 0.67          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 1        | 0.67          |
| (1,1794) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HG    | 16       | 0.67          |
| (1,1794) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HG    | 16       | 0.67          |
| (1,1794) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HG    | 16       | 0.67          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11  | 10       | 0.67          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12  | 10       | 0.67          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13  | 10       | 0.67          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11  | 16       | 0.67          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12  | 16       | 0.67          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13  | 16       | 0.67          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11  | 20       | 0.67          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12  | 20       | 0.67          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13  | 20       | 0.67          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11  | 20       | 0.67          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12  | 20       | 0.67          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13  | 20       | 0.67          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA    | 1        | 0.67          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA    | 1        | 0.67          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA    | 1        | 0.67          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11   | 17       | 0.67          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12   | 17       | 0.67          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13   | 17       | 0.67          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11   | 17       | 0.67          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12   | 17       | 0.67          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13   | 17       | 0.67          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 20       | 0.67          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 20       | 0.67          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 20       | 0.67          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 20       | 0.67          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 20       | 0.67          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 20       | 0.67          |
| (1,61)   | 1:86:A:LEU:HD11  | 1:78:A:SER:H     | 17       | 0.67          |
| (1,61)   | 1:86:A:LEU:HD12  | 1:78:A:SER:H     | 17       | 0.67          |
| (1,61)   | 1:86:A:LEU:HD13  | 1:78:A:SER:H     | 17       | 0.67          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA    | 2        | 0.67          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA    | 2        | 0.67          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA    | 2        | 0.67          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 6        | 0.66          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 6        | 0.66          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 6        | 0.66          |
| (1,3159) | 1:53:A:VAL:HG11  | 1:52:A:GLU:H     | 3        | 0.66          |
| (1,3159) | 1:53:A:VAL:HG12  | 1:52:A:GLU:H     | 3        | 0.66          |
| (1,3159) | 1:53:A:VAL:HG13  | 1:52:A:GLU:H     | 3        | 0.66          |
| (1,2575) | 1:123:A:VAL:HG21 | 1:124:A:GLU:HA   | 16       | 0.66          |
| (1,2575) | 1:123:A:VAL:HG22 | 1:124:A:GLU:HA   | 16       | 0.66          |
| (1,2575) | 1:123:A:VAL:HG23 | 1:124:A:GLU:HA   | 16       | 0.66          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 5        | 0.66          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 5        | 0.66          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 5        | 0.66          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 5        | 0.66          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 5        | 0.66          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 5        | 0.66          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 19       | 0.66          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 19       | 0.66          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 19       | 0.66          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 19       | 0.66          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 19       | 0.66          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 19       | 0.66          |
| (1,1216) | 1:53:A:VAL:HG21  | 1:52:A:GLU:HA    | 11       | 0.66          |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (1,1216) | 1:53:A:VAL:HG22  | 1:52:A:GLU:HA  | 11       | 0.66          |
| (1,1216) | 1:53:A:VAL:HG23  | 1:52:A:GLU:HA  | 11       | 0.66          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11 | 2        | 0.66          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12 | 2        | 0.66          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13 | 2        | 0.66          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11 | 2        | 0.66          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12 | 2        | 0.66          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13 | 2        | 0.66          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11 | 16       | 0.66          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12 | 16       | 0.66          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13 | 16       | 0.66          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11 | 16       | 0.66          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12 | 16       | 0.66          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13 | 16       | 0.66          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21 | 6        | 0.66          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22 | 6        | 0.66          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23 | 6        | 0.66          |
| (1,144)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HZ   | 11       | 0.66          |
| (1,144)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HZ   | 11       | 0.66          |
| (1,144)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HZ   | 11       | 0.66          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H   | 6        | 0.66          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H   | 6        | 0.66          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H   | 6        | 0.66          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2 | 9        | 0.66          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3 | 9        | 0.66          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2 | 9        | 0.66          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3 | 9        | 0.66          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2 | 9        | 0.66          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3 | 9        | 0.66          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2 | 9        | 0.66          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3 | 9        | 0.66          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2 | 9        | 0.66          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3 | 9        | 0.66          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2 | 9        | 0.66          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3 | 9        | 0.66          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H  | 20       | 0.65          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H  | 20       | 0.65          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H  | 20       | 0.65          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H  | 11       | 0.65          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H  | 11       | 0.65          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H  | 11       | 0.65          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H   | 20       | 0.65          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H    | 20       | 0.65          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H    | 20       | 0.65          |
| (1,1664) | 1:79:A:LEU:HD21  | 1:77:A:ILE:HA   | 10       | 0.65          |
| (1,1664) | 1:79:A:LEU:HD22  | 1:77:A:ILE:HA   | 10       | 0.65          |
| (1,1664) | 1:79:A:LEU:HD23  | 1:77:A:ILE:HA   | 10       | 0.65          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21 | 13       | 0.65          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG22 | 13       | 0.65          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG23 | 13       | 0.65          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11 | 12       | 0.65          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12 | 12       | 0.65          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13 | 12       | 0.65          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11 | 12       | 0.65          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12 | 12       | 0.65          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13 | 12       | 0.65          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 6        | 0.65          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 6        | 0.65          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 6        | 0.65          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA   | 18       | 0.65          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA   | 18       | 0.65          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA   | 18       | 0.65          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H   | 16       | 0.64          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H   | 16       | 0.64          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H   | 16       | 0.64          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H   | 5        | 0.64          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H   | 5        | 0.64          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H   | 5        | 0.64          |
| (1,2744) | 1:79:A:LEU:HD11  | 1:15:A:SER:HA   | 18       | 0.64          |
| (1,2744) | 1:79:A:LEU:HD12  | 1:15:A:SER:HA   | 18       | 0.64          |
| (1,2744) | 1:79:A:LEU:HD13  | 1:15:A:SER:HA   | 18       | 0.64          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 9        | 0.64          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 9        | 0.64          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 9        | 0.64          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 9        | 0.64          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 9        | 0.64          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 9        | 0.64          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 9        | 0.64          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 9        | 0.64          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 9        | 0.64          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 9        | 0.64          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 9        | 0.64          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 9        | 0.64          |
| (1,1794) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HG   | 8        | 0.64          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1794) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HG   | 8        | 0.64          |
| (1,1794) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HG   | 8        | 0.64          |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA   | 8        | 0.64          |
| (1,1776) | 1:37:A:LEU:HD12  | 1:86:A:LEU:HA   | 8        | 0.64          |
| (1,1776) | 1:37:A:LEU:HD13  | 1:86:A:LEU:HA   | 8        | 0.64          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD11 | 18       | 0.64          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD12 | 18       | 0.64          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD13 | 18       | 0.64          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21 | 9        | 0.64          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG22 | 9        | 0.64          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG23 | 9        | 0.64          |
| (1,1240) | 1:116:A:ARG:HG2  | 1:53:A:VAL:HG11 | 7        | 0.64          |
| (1,1240) | 1:116:A:ARG:HG2  | 1:53:A:VAL:HG12 | 7        | 0.64          |
| (1,1240) | 1:116:A:ARG:HG2  | 1:53:A:VAL:HG13 | 7        | 0.64          |
| (1,1240) | 1:116:A:ARG:HG3  | 1:53:A:VAL:HG11 | 7        | 0.64          |
| (1,1240) | 1:116:A:ARG:HG3  | 1:53:A:VAL:HG12 | 7        | 0.64          |
| (1,1240) | 1:116:A:ARG:HG3  | 1:53:A:VAL:HG13 | 7        | 0.64          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD11 | 8        | 0.64          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12 | 8        | 0.64          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13 | 8        | 0.64          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11 | 13       | 0.64          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG12 | 13       | 0.64          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG13 | 13       | 0.64          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 8        | 0.64          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 8        | 0.64          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 8        | 0.64          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 9        | 0.64          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 9        | 0.64          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 9        | 0.64          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ    | 4        | 0.64          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ    | 4        | 0.64          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ    | 4        | 0.64          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA   | 15       | 0.64          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA   | 15       | 0.64          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA   | 15       | 0.64          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H   | 12       | 0.63          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H   | 12       | 0.63          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H   | 12       | 0.63          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H   | 15       | 0.63          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H   | 15       | 0.63          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H   | 15       | 0.63          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H   | 18       | 0.63          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H   | 18       | 0.63          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H   | 18       | 0.63          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H    | 12       | 0.63          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H    | 12       | 0.63          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H    | 12       | 0.63          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11 | 1        | 0.63          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12 | 1        | 0.63          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13 | 1        | 0.63          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB2  | 11       | 0.63          |
| (1,516)  | 1:32:A:VAL:HG11  | 1:19:A:GLU:HB3  | 11       | 0.63          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB2  | 11       | 0.63          |
| (1,516)  | 1:32:A:VAL:HG12  | 1:19:A:GLU:HB3  | 11       | 0.63          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB2  | 11       | 0.63          |
| (1,516)  | 1:32:A:VAL:HG13  | 1:19:A:GLU:HB3  | 11       | 0.63          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11  | 13       | 0.63          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12  | 13       | 0.63          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13  | 13       | 0.63          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11  | 13       | 0.63          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12  | 13       | 0.63          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13  | 13       | 0.63          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ    | 1        | 0.63          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ    | 1        | 0.63          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ    | 1        | 0.63          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ    | 9        | 0.63          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ    | 9        | 0.63          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ    | 9        | 0.63          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA   | 4        | 0.63          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA   | 4        | 0.63          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA   | 4        | 0.63          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H   | 20       | 0.62          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H   | 20       | 0.62          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H   | 20       | 0.62          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 1        | 0.62          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 1        | 0.62          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 1        | 0.62          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11 | 14       | 0.62          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12 | 14       | 0.62          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13 | 14       | 0.62          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11 | 14       | 0.62          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12 | 14       | 0.62          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13 | 14       | 0.62          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ    | 15       | 0.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ     | 15       | 0.62          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ     | 15       | 0.62          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 14       | 0.62          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 14       | 0.62          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 14       | 0.62          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 14       | 0.62          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 14       | 0.62          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 14       | 0.62          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H     | 11       | 0.62          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H     | 11       | 0.62          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H     | 11       | 0.62          |
| (1,3538) | 1:115:A:VAL:HG11 | 1:112:A:PHE:H    | 1        | 0.61          |
| (1,3538) | 1:115:A:VAL:HG12 | 1:112:A:PHE:H    | 1        | 0.61          |
| (1,3538) | 1:115:A:VAL:HG13 | 1:112:A:PHE:H    | 1        | 0.61          |
| (1,3472) | 1:79:A:LEU:HD21  | 1:99:A:TRP:H     | 15       | 0.61          |
| (1,3472) | 1:79:A:LEU:HD22  | 1:99:A:TRP:H     | 15       | 0.61          |
| (1,3472) | 1:79:A:LEU:HD23  | 1:99:A:TRP:H     | 15       | 0.61          |
| (1,2744) | 1:79:A:LEU:HD11  | 1:15:A:SER:HA    | 15       | 0.61          |
| (1,2744) | 1:79:A:LEU:HD12  | 1:15:A:SER:HA    | 15       | 0.61          |
| (1,2744) | 1:79:A:LEU:HD13  | 1:15:A:SER:HA    | 15       | 0.61          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 5        | 0.61          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 5        | 0.61          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 5        | 0.61          |
| (1,1794) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HG    | 10       | 0.61          |
| (1,1794) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HG    | 10       | 0.61          |
| (1,1794) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HG    | 10       | 0.61          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD11  | 15       | 0.61          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD12  | 15       | 0.61          |
| (1,1738) | 1:15:A:SER:HA    | 1:79:A:LEU:HD13  | 15       | 0.61          |
| (1,1664) | 1:79:A:LEU:HD21  | 1:77:A:ILE:HA    | 18       | 0.61          |
| (1,1664) | 1:79:A:LEU:HD22  | 1:77:A:ILE:HA    | 18       | 0.61          |
| (1,1664) | 1:79:A:LEU:HD23  | 1:77:A:ILE:HA    | 18       | 0.61          |
| (1,1216) | 1:53:A:VAL:HG21  | 1:52:A:GLU:HA    | 14       | 0.61          |
| (1,1216) | 1:53:A:VAL:HG22  | 1:52:A:GLU:HA    | 14       | 0.61          |
| (1,1216) | 1:53:A:VAL:HG23  | 1:52:A:GLU:HA    | 14       | 0.61          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD21  | 10       | 0.61          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD22  | 10       | 0.61          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD23  | 10       | 0.61          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD21  | 10       | 0.61          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD22  | 10       | 0.61          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD23  | 10       | 0.61          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21  | 10       | 0.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22  | 10       | 0.61          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23  | 10       | 0.61          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21  | 10       | 0.61          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22  | 10       | 0.61          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23  | 10       | 0.61          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21  | 10       | 0.61          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22  | 10       | 0.61          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23  | 10       | 0.61          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11  | 4        | 0.61          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12  | 4        | 0.61          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13  | 4        | 0.61          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11  | 15       | 0.61          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12  | 15       | 0.61          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13  | 15       | 0.61          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA    | 5        | 0.61          |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA    | 5        | 0.61          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA    | 5        | 0.61          |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG11   | 17       | 0.61          |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG12   | 17       | 0.61          |
| (1,254)  | 1:99:A:TRP:HH2   | 1:4:A:VAL:HG13   | 17       | 0.61          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 1        | 0.61          |
| (1,49)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 1        | 0.61          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 1        | 0.61          |
| (1,49)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 1        | 0.61          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 1        | 0.61          |
| (1,49)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 1        | 0.61          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2   | 1        | 0.61          |
| (1,47)   | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3   | 1        | 0.61          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2   | 1        | 0.61          |
| (1,47)   | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3   | 1        | 0.61          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2   | 1        | 0.61          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3   | 1        | 0.61          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA    | 13       | 0.61          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA    | 13       | 0.61          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA    | 13       | 0.61          |
| (1,2434) | 1:79:A:LEU:HD21  | 1:119:A:VAL:HG21 | 1        | 0.6           |
| (1,2434) | 1:79:A:LEU:HD21  | 1:119:A:VAL:HG22 | 1        | 0.6           |
| (1,2434) | 1:79:A:LEU:HD21  | 1:119:A:VAL:HG23 | 1        | 0.6           |
| (1,2434) | 1:79:A:LEU:HD22  | 1:119:A:VAL:HG21 | 1        | 0.6           |
| (1,2434) | 1:79:A:LEU:HD22  | 1:119:A:VAL:HG22 | 1        | 0.6           |
| (1,2434) | 1:79:A:LEU:HD22  | 1:119:A:VAL:HG23 | 1        | 0.6           |
| (1,2434) | 1:79:A:LEU:HD23  | 1:119:A:VAL:HG21 | 1        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2434) | 1:79:A:LEU:HD23  | 1:119:A:VAL:HG22 | 1        | 0.6           |
| (1,2434) | 1:79:A:LEU:HD23  | 1:119:A:VAL:HG23 | 1        | 0.6           |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD11  | 13       | 0.6           |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD12  | 13       | 0.6           |
| (1,911)  | 1:65:A:ILE:HB    | 1:37:A:LEU:HD13  | 13       | 0.6           |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21  | 2        | 0.6           |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22  | 2        | 0.6           |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23  | 2        | 0.6           |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21  | 2        | 0.6           |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22  | 2        | 0.6           |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23  | 2        | 0.6           |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21  | 2        | 0.6           |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22  | 2        | 0.6           |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23  | 2        | 0.6           |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21  | 12       | 0.6           |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22  | 12       | 0.6           |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23  | 12       | 0.6           |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21  | 12       | 0.6           |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22  | 12       | 0.6           |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23  | 12       | 0.6           |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21  | 12       | 0.6           |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22  | 12       | 0.6           |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23  | 12       | 0.6           |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11   | 14       | 0.6           |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12   | 14       | 0.6           |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13   | 14       | 0.6           |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11   | 14       | 0.6           |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12   | 14       | 0.6           |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13   | 14       | 0.6           |
| (1,2124) | 1:4:A:VAL:HG21   | 1:126:A:LEU:HG   | 6        | 0.59          |
| (1,2124) | 1:4:A:VAL:HG22   | 1:126:A:LEU:HG   | 6        | 0.59          |
| (1,2124) | 1:4:A:VAL:HG23   | 1:126:A:LEU:HG   | 6        | 0.59          |
| (1,2084) | 1:79:A:LEU:HD21  | 1:101:A:LEU:HG   | 18       | 0.59          |
| (1,2084) | 1:79:A:LEU:HD22  | 1:101:A:LEU:HG   | 18       | 0.59          |
| (1,2084) | 1:79:A:LEU:HD23  | 1:101:A:LEU:HG   | 18       | 0.59          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG21  | 13       | 0.59          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG22  | 13       | 0.59          |
| (1,1960) | 1:126:A:LEU:HD11 | 1:95:A:ILE:HG23  | 13       | 0.59          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG21  | 13       | 0.59          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG22  | 13       | 0.59          |
| (1,1960) | 1:126:A:LEU:HD12 | 1:95:A:ILE:HG23  | 13       | 0.59          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG21  | 13       | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG22  | 13       | 0.59          |
| (1,1960) | 1:126:A:LEU:HD13 | 1:95:A:ILE:HG23  | 13       | 0.59          |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA    | 2        | 0.59          |
| (1,1776) | 1:37:A:LEU:HD12  | 1:86:A:LEU:HA    | 2        | 0.59          |
| (1,1776) | 1:37:A:LEU:HD13  | 1:86:A:LEU:HA    | 2        | 0.59          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11  | 18       | 0.59          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12  | 18       | 0.59          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13  | 18       | 0.59          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11  | 18       | 0.59          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12  | 18       | 0.59          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13  | 18       | 0.59          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD11  | 2        | 0.59          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12  | 2        | 0.59          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13  | 2        | 0.59          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21  | 13       | 0.59          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22  | 13       | 0.59          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23  | 13       | 0.59          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21  | 13       | 0.59          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22  | 13       | 0.59          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23  | 13       | 0.59          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21  | 13       | 0.59          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22  | 13       | 0.59          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23  | 13       | 0.59          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ     | 18       | 0.59          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ     | 18       | 0.59          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ     | 18       | 0.59          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 6        | 0.58          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 6        | 0.58          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 6        | 0.58          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 7        | 0.58          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 7        | 0.58          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 7        | 0.58          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 9        | 0.58          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 9        | 0.58          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 9        | 0.58          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 12       | 0.58          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 12       | 0.58          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 12       | 0.58          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG11 | 13       | 0.58          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG12 | 13       | 0.58          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG13 | 13       | 0.58          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21  | 1        | 0.58          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG22  | 1        | 0.58          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG23  | 1        | 0.58          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG21  | 5        | 0.58          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG22  | 5        | 0.58          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG23  | 5        | 0.58          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG21  | 15       | 0.58          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG22  | 15       | 0.58          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG23  | 15       | 0.58          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG21  | 20       | 0.58          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG22  | 20       | 0.58          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG23  | 20       | 0.58          |
| (1,313)  | 1:5:A:MET:HG2   | 1:7:A:VAL:HG11   | 3        | 0.58          |
| (1,313)  | 1:5:A:MET:HG2   | 1:7:A:VAL:HG12   | 3        | 0.58          |
| (1,313)  | 1:5:A:MET:HG2   | 1:7:A:VAL:HG13   | 3        | 0.58          |
| (1,313)  | 1:5:A:MET:HG3   | 1:7:A:VAL:HG11   | 3        | 0.58          |
| (1,313)  | 1:5:A:MET:HG3   | 1:7:A:VAL:HG12   | 3        | 0.58          |
| (1,313)  | 1:5:A:MET:HG3   | 1:7:A:VAL:HG13   | 3        | 0.58          |
| (1,44)   | 1:86:A:LEU:HD11 | 1:87:A:PRO:HB2   | 12       | 0.58          |
| (1,44)   | 1:86:A:LEU:HD11 | 1:87:A:PRO:HB3   | 12       | 0.58          |
| (1,44)   | 1:86:A:LEU:HD12 | 1:87:A:PRO:HB2   | 12       | 0.58          |
| (1,44)   | 1:86:A:LEU:HD12 | 1:87:A:PRO:HB3   | 12       | 0.58          |
| (1,44)   | 1:86:A:LEU:HD13 | 1:87:A:PRO:HB2   | 12       | 0.58          |
| (1,44)   | 1:86:A:LEU:HD13 | 1:87:A:PRO:HB3   | 12       | 0.58          |
| (1,41)   | 1:91:A:VAL:HG11 | 1:90:A:TRP:HA    | 12       | 0.58          |
| (1,41)   | 1:91:A:VAL:HG12 | 1:90:A:TRP:HA    | 12       | 0.58          |
| (1,41)   | 1:91:A:VAL:HG13 | 1:90:A:TRP:HA    | 12       | 0.58          |
| (1,3472) | 1:79:A:LEU:HD21 | 1:99:A:TRP:H     | 18       | 0.57          |
| (1,3472) | 1:79:A:LEU:HD22 | 1:99:A:TRP:H     | 18       | 0.57          |
| (1,3472) | 1:79:A:LEU:HD23 | 1:99:A:TRP:H     | 18       | 0.57          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG11 | 9        | 0.57          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG12 | 9        | 0.57          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG13 | 9        | 0.57          |
| (1,1776) | 1:37:A:LEU:HD11 | 1:86:A:LEU:HA    | 12       | 0.57          |
| (1,1776) | 1:37:A:LEU:HD12 | 1:86:A:LEU:HA    | 12       | 0.57          |
| (1,1776) | 1:37:A:LEU:HD13 | 1:86:A:LEU:HA    | 12       | 0.57          |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG11  | 18       | 0.57          |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG12  | 18       | 0.57          |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG13  | 18       | 0.57          |
| (1,1216) | 1:53:A:VAL:HG21 | 1:52:A:GLU:HA    | 13       | 0.57          |
| (1,1216) | 1:53:A:VAL:HG22 | 1:52:A:GLU:HA    | 13       | 0.57          |
| (1,1216) | 1:53:A:VAL:HG23 | 1:52:A:GLU:HA    | 13       | 0.57          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD11  | 12       | 0.57          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,917) | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12 | 12       | 0.57          |
| (1,917) | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13 | 12       | 0.57          |
| (1,812) | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21 | 4        | 0.57          |
| (1,812) | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22 | 4        | 0.57          |
| (1,812) | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23 | 4        | 0.57          |
| (1,812) | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21 | 4        | 0.57          |
| (1,812) | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22 | 4        | 0.57          |
| (1,812) | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23 | 4        | 0.57          |
| (1,812) | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21 | 4        | 0.57          |
| (1,812) | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22 | 4        | 0.57          |
| (1,812) | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23 | 4        | 0.57          |
| (1,807) | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 2        | 0.57          |
| (1,807) | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 2        | 0.57          |
| (1,807) | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 2        | 0.57          |
| (1,807) | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 18       | 0.57          |
| (1,807) | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 18       | 0.57          |
| (1,807) | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 18       | 0.57          |
| (1,313) | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11  | 4        | 0.57          |
| (1,313) | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12  | 4        | 0.57          |
| (1,313) | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13  | 4        | 0.57          |
| (1,313) | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11  | 4        | 0.57          |
| (1,313) | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12  | 4        | 0.57          |
| (1,313) | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13  | 4        | 0.57          |
| (1,145) | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ    | 13       | 0.57          |
| (1,145) | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ    | 13       | 0.57          |
| (1,145) | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ    | 13       | 0.57          |
| (1,142) | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE1   | 10       | 0.57          |
| (1,142) | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE2   | 10       | 0.57          |
| (1,142) | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE1   | 10       | 0.57          |
| (1,142) | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE2   | 10       | 0.57          |
| (1,142) | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE1   | 10       | 0.57          |
| (1,142) | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE2   | 10       | 0.57          |
| (1,49)  | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2  | 10       | 0.57          |
| (1,49)  | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3  | 10       | 0.57          |
| (1,49)  | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2  | 10       | 0.57          |
| (1,49)  | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3  | 10       | 0.57          |
| (1,49)  | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2  | 10       | 0.57          |
| (1,49)  | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3  | 10       | 0.57          |
| (1,47)  | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG2  | 10       | 0.57          |
| (1,47)  | 1:37:A:LEU:HD11  | 1:87:A:PRO:HG3  | 10       | 0.57          |
| (1,47)  | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG2  | 10       | 0.57          |
| (1,47)  | 1:37:A:LEU:HD12  | 1:87:A:PRO:HG3  | 10       | 0.57          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG2  | 10       | 0.57          |
| (1,47)   | 1:37:A:LEU:HD13  | 1:87:A:PRO:HG3  | 10       | 0.57          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA   | 7        | 0.57          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA   | 7        | 0.57          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA   | 7        | 0.57          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA   | 15       | 0.57          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA   | 15       | 0.57          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA   | 15       | 0.57          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA   | 20       | 0.57          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA   | 20       | 0.57          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA   | 20       | 0.57          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H   | 1        | 0.56          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H   | 1        | 0.56          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H   | 1        | 0.56          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H   | 3        | 0.56          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H   | 3        | 0.56          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H   | 3        | 0.56          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H   | 8        | 0.56          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H   | 8        | 0.56          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H   | 8        | 0.56          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H   | 19       | 0.56          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H   | 19       | 0.56          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H   | 19       | 0.56          |
| (1,3472) | 1:79:A:LEU:HD21  | 1:99:A:TRP:H    | 10       | 0.56          |
| (1,3472) | 1:79:A:LEU:HD22  | 1:99:A:TRP:H    | 10       | 0.56          |
| (1,3472) | 1:79:A:LEU:HD23  | 1:99:A:TRP:H    | 10       | 0.56          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21 | 3        | 0.56          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22 | 3        | 0.56          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23 | 3        | 0.56          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21 | 3        | 0.56          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22 | 3        | 0.56          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23 | 3        | 0.56          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21 | 3        | 0.56          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22 | 3        | 0.56          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23 | 3        | 0.56          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11 | 3        | 0.56          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12 | 3        | 0.56          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13 | 3        | 0.56          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11 | 3        | 0.56          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12 | 3        | 0.56          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13 | 3        | 0.56          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG21  | 8        | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG22   | 8        | 0.56          |
| (1,271)  | 1:6:A:PHE:HE1    | 1:4:A:VAL:HG23   | 8        | 0.56          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG21   | 8        | 0.56          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG22   | 8        | 0.56          |
| (1,271)  | 1:6:A:PHE:HE2    | 1:4:A:VAL:HG23   | 8        | 0.56          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 3        | 0.56          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 3        | 0.56          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 3        | 0.56          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 3        | 0.56          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 3        | 0.56          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 3        | 0.56          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 2        | 0.55          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 2        | 0.55          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 2        | 0.55          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 2        | 0.55          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 2        | 0.55          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 2        | 0.55          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 2        | 0.55          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 2        | 0.55          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 2        | 0.55          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 2        | 0.55          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 2        | 0.55          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 2        | 0.55          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 17       | 0.55          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 17       | 0.55          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 17       | 0.55          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 12       | 0.55          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 12       | 0.55          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 12       | 0.55          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 4        | 0.55          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 4        | 0.55          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 4        | 0.55          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 4        | 0.55          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 4        | 0.55          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 4        | 0.55          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 12       | 0.55          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 12       | 0.55          |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 12       | 0.55          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 12       | 0.55          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 12       | 0.55          |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 12       | 0.55          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11  | 16       | 0.55          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12 | 16       | 0.55          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13 | 16       | 0.55          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11 | 7        | 0.55          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12 | 7        | 0.55          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13 | 7        | 0.55          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11 | 7        | 0.55          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12 | 7        | 0.55          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13 | 7        | 0.55          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA   | 12       | 0.55          |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA   | 12       | 0.55          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA   | 12       | 0.55          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11  | 8        | 0.55          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12  | 8        | 0.55          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13  | 8        | 0.55          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11  | 8        | 0.55          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12  | 8        | 0.55          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13  | 8        | 0.55          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11  | 19       | 0.55          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12  | 19       | 0.55          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13  | 19       | 0.55          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11  | 19       | 0.55          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12  | 19       | 0.55          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13  | 19       | 0.55          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21  | 11       | 0.55          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22  | 11       | 0.55          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23  | 11       | 0.55          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ    | 8        | 0.55          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ    | 8        | 0.55          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ    | 8        | 0.55          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2  | 14       | 0.55          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3  | 14       | 0.55          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2  | 14       | 0.55          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3  | 14       | 0.55          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2  | 14       | 0.55          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3  | 14       | 0.55          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA   | 1        | 0.55          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA   | 1        | 0.55          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA   | 1        | 0.55          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA   | 14       | 0.55          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA   | 14       | 0.55          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA   | 14       | 0.55          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H   | 19       | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 19       | 0.54          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 19       | 0.54          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 2        | 0.54          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 2        | 0.54          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 2        | 0.54          |
| (1,1794) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HG    | 11       | 0.54          |
| (1,1794) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HG    | 11       | 0.54          |
| (1,1794) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HG    | 11       | 0.54          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 12       | 0.54          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 12       | 0.54          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 12       | 0.54          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 20       | 0.54          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 20       | 0.54          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 20       | 0.54          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ     | 2        | 0.54          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ     | 2        | 0.54          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ     | 2        | 0.54          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H     | 12       | 0.54          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H     | 12       | 0.54          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H     | 12       | 0.54          |
| (1,41)   | 1:91:A:VAL:HG11  | 1:90:A:TRP:HA    | 19       | 0.54          |
| (1,41)   | 1:91:A:VAL:HG12  | 1:90:A:TRP:HA    | 19       | 0.54          |
| (1,41)   | 1:91:A:VAL:HG13  | 1:90:A:TRP:HA    | 19       | 0.54          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 12       | 0.53          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 12       | 0.53          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 12       | 0.53          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 12       | 0.53          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 12       | 0.53          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 12       | 0.53          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 12       | 0.53          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 12       | 0.53          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 12       | 0.53          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 12       | 0.53          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 12       | 0.53          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 12       | 0.53          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 4        | 0.53          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 4        | 0.53          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 4        | 0.53          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 13       | 0.53          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 13       | 0.53          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 13       | 0.53          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 13       | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 13       | 0.53          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 13       | 0.53          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 17       | 0.53          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG12 | 17       | 0.53          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG13 | 17       | 0.53          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 16       | 0.53          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 16       | 0.53          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 16       | 0.53          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 16       | 0.53          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 16       | 0.53          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 16       | 0.53          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 16       | 0.53          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 16       | 0.53          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 16       | 0.53          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 16       | 0.53          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 16       | 0.53          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 16       | 0.53          |
| (1,2084) | 1:79:A:LEU:HD21  | 1:101:A:LEU:HG   | 15       | 0.53          |
| (1,2084) | 1:79:A:LEU:HD22  | 1:101:A:LEU:HG   | 15       | 0.53          |
| (1,2084) | 1:79:A:LEU:HD23  | 1:101:A:LEU:HG   | 15       | 0.53          |
| (1,1664) | 1:79:A:LEU:HD21  | 1:77:A:ILE:HA    | 8        | 0.53          |
| (1,1664) | 1:79:A:LEU:HD22  | 1:77:A:ILE:HA    | 8        | 0.53          |
| (1,1664) | 1:79:A:LEU:HD23  | 1:77:A:ILE:HA    | 8        | 0.53          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21  | 4        | 0.53          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG22  | 4        | 0.53          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG23  | 4        | 0.53          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21  | 12       | 0.53          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG22  | 12       | 0.53          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG23  | 12       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21  | 15       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22  | 15       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23  | 15       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21  | 15       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22  | 15       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23  | 15       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21  | 15       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22  | 15       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23  | 15       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21  | 18       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22  | 18       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23  | 18       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21  | 18       | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22  | 18       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23  | 18       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21  | 18       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22  | 18       | 0.53          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23  | 18       | 0.53          |
| (1,142)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE1    | 11       | 0.53          |
| (1,142)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE2    | 11       | 0.53          |
| (1,142)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE1    | 11       | 0.53          |
| (1,142)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE2    | 11       | 0.53          |
| (1,142)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE1    | 11       | 0.53          |
| (1,142)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE2    | 11       | 0.53          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 13       | 0.52          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 13       | 0.52          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 13       | 0.52          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 16       | 0.52          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 16       | 0.52          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 16       | 0.52          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 5        | 0.52          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 5        | 0.52          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 5        | 0.52          |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG11 | 19       | 0.52          |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG12 | 19       | 0.52          |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG13 | 19       | 0.52          |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG11 | 19       | 0.52          |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG12 | 19       | 0.52          |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG13 | 19       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 13       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 13       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 13       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 13       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 13       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 13       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 15       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 15       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 15       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 15       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 15       | 0.52          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 15       | 0.52          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 13       | 0.52          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 13       | 0.52          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 13       | 0.52          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 13       | 0.52          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 13       | 0.52          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 13       | 0.52          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2 | 15       | 0.52          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3 | 15       | 0.52          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2 | 15       | 0.52          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3 | 15       | 0.52          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2 | 15       | 0.52          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3 | 15       | 0.52          |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD11 | 8        | 0.52          |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD12 | 8        | 0.52          |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD13 | 8        | 0.52          |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD11 | 8        | 0.52          |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD12 | 8        | 0.52          |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD13 | 8        | 0.52          |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD11 | 8        | 0.52          |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD12 | 8        | 0.52          |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD13 | 8        | 0.52          |
| (1,1755) | 1:91:A:VAL:HG21  | 1:83:A:GLY:HA2  | 16       | 0.52          |
| (1,1755) | 1:91:A:VAL:HG21  | 1:83:A:GLY:HA3  | 16       | 0.52          |
| (1,1755) | 1:91:A:VAL:HG22  | 1:83:A:GLY:HA2  | 16       | 0.52          |
| (1,1755) | 1:91:A:VAL:HG22  | 1:83:A:GLY:HA3  | 16       | 0.52          |
| (1,1755) | 1:91:A:VAL:HG23  | 1:83:A:GLY:HA2  | 16       | 0.52          |
| (1,1755) | 1:91:A:VAL:HG23  | 1:83:A:GLY:HA3  | 16       | 0.52          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21 | 14       | 0.52          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22 | 14       | 0.52          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23 | 14       | 0.52          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21 | 14       | 0.52          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22 | 14       | 0.52          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23 | 14       | 0.52          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21 | 14       | 0.52          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22 | 14       | 0.52          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23 | 14       | 0.52          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG11 | 11       | 0.52          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG12 | 11       | 0.52          |
| (1,807)  | 1:6:A:PHE:H      | 1:32:A:VAL:HG13 | 11       | 0.52          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11  | 1        | 0.52          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12  | 1        | 0.52          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13  | 1        | 0.52          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11  | 1        | 0.52          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12  | 1        | 0.52          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13  | 1        | 0.52          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21  | 5        | 0.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22   | 5        | 0.52          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23   | 5        | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 3        | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 3        | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 3        | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 10       | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 10       | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 10       | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 14       | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 14       | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 14       | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 15       | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 15       | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 15       | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 19       | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 19       | 0.52          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 19       | 0.52          |
| (1,264)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG21   | 13       | 0.52          |
| (1,264)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG22   | 13       | 0.52          |
| (1,264)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG23   | 13       | 0.52          |
| (1,264)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG21   | 13       | 0.52          |
| (1,264)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG22   | 13       | 0.52          |
| (1,264)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG23   | 13       | 0.52          |
| (1,264)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG21   | 13       | 0.52          |
| (1,264)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG22   | 13       | 0.52          |
| (1,264)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG23   | 13       | 0.52          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H     | 13       | 0.52          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H     | 13       | 0.52          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H     | 13       | 0.52          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 14       | 0.51          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 14       | 0.51          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 14       | 0.51          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB2  | 6        | 0.51          |
| (1,2670) | 1:115:A:VAL:HG21 | 1:102:A:GLU:HB3  | 6        | 0.51          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB2  | 6        | 0.51          |
| (1,2670) | 1:115:A:VAL:HG22 | 1:102:A:GLU:HB3  | 6        | 0.51          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB2  | 6        | 0.51          |
| (1,2670) | 1:115:A:VAL:HG23 | 1:102:A:GLU:HB3  | 6        | 0.51          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 17       | 0.51          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 17       | 0.51          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 17       | 0.51          |
| (1,1756) | 1:86:A:LEU:HD11  | 1:84:A:VAL:HA    | 19       | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1756) | 1:86:A:LEU:HD12  | 1:84:A:VAL:HA    | 19       | 0.51          |
| (1,1756) | 1:86:A:LEU:HD13  | 1:84:A:VAL:HA    | 19       | 0.51          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21  | 8        | 0.51          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG22  | 8        | 0.51          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG23  | 8        | 0.51          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD21  | 1        | 0.51          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD22  | 1        | 0.51          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD23  | 1        | 0.51          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD21  | 1        | 0.51          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD22  | 1        | 0.51          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD23  | 1        | 0.51          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 11       | 0.51          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 11       | 0.51          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 11       | 0.51          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 11       | 0.51          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 11       | 0.51          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 11       | 0.51          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 15       | 0.51          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 15       | 0.51          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 15       | 0.51          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 15       | 0.51          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 15       | 0.51          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 15       | 0.51          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21  | 1        | 0.51          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22  | 1        | 0.51          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23  | 1        | 0.51          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21  | 1        | 0.51          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22  | 1        | 0.51          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23  | 1        | 0.51          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21  | 1        | 0.51          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22  | 1        | 0.51          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23  | 1        | 0.51          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11  | 15       | 0.51          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12  | 15       | 0.51          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13  | 15       | 0.51          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11  | 15       | 0.51          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12  | 15       | 0.51          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13  | 15       | 0.51          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA    | 17       | 0.51          |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA    | 17       | 0.51          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA    | 17       | 0.51          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG21   | 15       | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG22   | 15       | 0.51          |
| (1,323)  | 1:86:A:LEU:HA    | 1:7:A:VAL:HG23   | 15       | 0.51          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 2        | 0.51          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 2        | 0.51          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 2        | 0.51          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 16       | 0.51          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 16       | 0.51          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 16       | 0.51          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 15       | 0.51          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 15       | 0.51          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 15       | 0.51          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 15       | 0.51          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 15       | 0.51          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 15       | 0.51          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 15       | 0.5           |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 15       | 0.5           |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 15       | 0.5           |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 15       | 0.5           |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 15       | 0.5           |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 15       | 0.5           |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 15       | 0.5           |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 15       | 0.5           |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 15       | 0.5           |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 15       | 0.5           |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 15       | 0.5           |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 15       | 0.5           |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 15       | 0.5           |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 15       | 0.5           |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 15       | 0.5           |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG11 | 16       | 0.5           |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG12 | 16       | 0.5           |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG13 | 16       | 0.5           |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA    | 13       | 0.5           |
| (1,1776) | 1:37:A:LEU:HD12  | 1:86:A:LEU:HA    | 13       | 0.5           |
| (1,1776) | 1:37:A:LEU:HD13  | 1:86:A:LEU:HA    | 13       | 0.5           |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA    | 16       | 0.5           |
| (1,1776) | 1:37:A:LEU:HD12  | 1:86:A:LEU:HA    | 16       | 0.5           |
| (1,1776) | 1:37:A:LEU:HD13  | 1:86:A:LEU:HA    | 16       | 0.5           |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21  | 7        | 0.5           |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG22  | 7        | 0.5           |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG23  | 7        | 0.5           |
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG21  | 13       | 0.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG22  | 13       | 0.5           |
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG23  | 13       | 0.5           |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG21  | 13       | 0.5           |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG22  | 13       | 0.5           |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG23  | 13       | 0.5           |
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG21  | 13       | 0.5           |
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG22  | 13       | 0.5           |
| (1,1250) | 1:52:A:GLU:HB2   | 1:53:A:VAL:HG23  | 13       | 0.5           |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG21  | 13       | 0.5           |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG22  | 13       | 0.5           |
| (1,1250) | 1:52:A:GLU:HB3   | 1:53:A:VAL:HG23  | 13       | 0.5           |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD11  | 13       | 0.5           |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12  | 13       | 0.5           |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13  | 13       | 0.5           |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD11  | 16       | 0.5           |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12  | 16       | 0.5           |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13  | 16       | 0.5           |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11   | 6        | 0.5           |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12   | 6        | 0.5           |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13   | 6        | 0.5           |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11   | 6        | 0.5           |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12   | 6        | 0.5           |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13   | 6        | 0.5           |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 8        | 0.5           |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 8        | 0.5           |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 8        | 0.5           |
| (1,243)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HB     | 6        | 0.5           |
| (1,243)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HB     | 6        | 0.5           |
| (1,243)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HB     | 6        | 0.5           |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ     | 3        | 0.5           |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ     | 3        | 0.5           |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ     | 3        | 0.5           |
| (1,144)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HZ     | 15       | 0.5           |
| (1,144)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HZ     | 15       | 0.5           |
| (1,144)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HZ     | 15       | 0.5           |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 14       | 0.49          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 14       | 0.49          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 14       | 0.49          |
| (1,3349) | 1:4:A:VAL:HG21   | 1:77:A:ILE:H     | 1        | 0.49          |
| (1,3349) | 1:4:A:VAL:HG22   | 1:77:A:ILE:H     | 1        | 0.49          |
| (1,3349) | 1:4:A:VAL:HG23   | 1:77:A:ILE:H     | 1        | 0.49          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 8        | 0.49          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2566) | 1:119:A:VAL:HA  | 1:123:A:VAL:HG12 | 8        | 0.49          |
| (1,2566) | 1:119:A:VAL:HA  | 1:123:A:VAL:HG13 | 8        | 0.49          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG11 | 11       | 0.49          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG12 | 11       | 0.49          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG13 | 11       | 0.49          |
| (1,2434) | 1:79:A:LEU:HD21 | 1:119:A:VAL:HG21 | 20       | 0.49          |
| (1,2434) | 1:79:A:LEU:HD21 | 1:119:A:VAL:HG22 | 20       | 0.49          |
| (1,2434) | 1:79:A:LEU:HD21 | 1:119:A:VAL:HG23 | 20       | 0.49          |
| (1,2434) | 1:79:A:LEU:HD22 | 1:119:A:VAL:HG21 | 20       | 0.49          |
| (1,2434) | 1:79:A:LEU:HD22 | 1:119:A:VAL:HG22 | 20       | 0.49          |
| (1,2434) | 1:79:A:LEU:HD22 | 1:119:A:VAL:HG23 | 20       | 0.49          |
| (1,2434) | 1:79:A:LEU:HD23 | 1:119:A:VAL:HG21 | 20       | 0.49          |
| (1,2434) | 1:79:A:LEU:HD23 | 1:119:A:VAL:HG22 | 20       | 0.49          |
| (1,2434) | 1:79:A:LEU:HD23 | 1:119:A:VAL:HG23 | 20       | 0.49          |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG11  | 20       | 0.49          |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG12  | 20       | 0.49          |
| (1,1761) | 1:82:A:CYS:H    | 1:84:A:VAL:HG13  | 20       | 0.49          |
| (1,1240) | 1:116:A:ARG:HG2 | 1:53:A:VAL:HG11  | 17       | 0.49          |
| (1,1240) | 1:116:A:ARG:HG2 | 1:53:A:VAL:HG12  | 17       | 0.49          |
| (1,1240) | 1:116:A:ARG:HG2 | 1:53:A:VAL:HG13  | 17       | 0.49          |
| (1,1240) | 1:116:A:ARG:HG3 | 1:53:A:VAL:HG11  | 17       | 0.49          |
| (1,1240) | 1:116:A:ARG:HG3 | 1:53:A:VAL:HG12  | 17       | 0.49          |
| (1,1240) | 1:116:A:ARG:HG3 | 1:53:A:VAL:HG13  | 17       | 0.49          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG11  | 4        | 0.49          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG12  | 4        | 0.49          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG13  | 4        | 0.49          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG11  | 4        | 0.49          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG12  | 4        | 0.49          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG13  | 4        | 0.49          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG11  | 15       | 0.49          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG12  | 15       | 0.49          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG13  | 15       | 0.49          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG11  | 15       | 0.49          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG12  | 15       | 0.49          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG13  | 15       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG21  | 19       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG22  | 19       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG23  | 19       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG21  | 19       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG22  | 19       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG23  | 19       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG23  | 1:32:A:VAL:HG21  | 19       | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22  | 19       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23  | 19       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG21  | 20       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG22  | 20       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG21   | 1:32:A:VAL:HG23  | 20       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG21  | 20       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG22  | 20       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG22   | 1:32:A:VAL:HG23  | 20       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG21  | 20       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG22  | 20       | 0.49          |
| (1,812)  | 1:4:A:VAL:HG23   | 1:32:A:VAL:HG23  | 20       | 0.49          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB1   | 16       | 0.49          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB2   | 16       | 0.49          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB3   | 16       | 0.49          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB1   | 16       | 0.49          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB2   | 16       | 0.49          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB3   | 16       | 0.49          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB1   | 16       | 0.49          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB2   | 16       | 0.49          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB3   | 16       | 0.49          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11   | 20       | 0.49          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12   | 20       | 0.49          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13   | 20       | 0.49          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11   | 20       | 0.49          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12   | 20       | 0.49          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13   | 20       | 0.49          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG21   | 1        | 0.49          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG22   | 1        | 0.49          |
| (1,276)  | 1:77:A:ILE:H     | 1:4:A:VAL:HG23   | 1        | 0.49          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 18       | 0.49          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 18       | 0.49          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 18       | 0.49          |
| (1,142)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE1    | 15       | 0.49          |
| (1,142)  | 1:123:A:VAL:HG11 | 1:6:A:PHE:HE2    | 15       | 0.49          |
| (1,142)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE1    | 15       | 0.49          |
| (1,142)  | 1:123:A:VAL:HG12 | 1:6:A:PHE:HE2    | 15       | 0.49          |
| (1,142)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE1    | 15       | 0.49          |
| (1,142)  | 1:123:A:VAL:HG13 | 1:6:A:PHE:HE2    | 15       | 0.49          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 13       | 0.48          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 13       | 0.48          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 13       | 0.48          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 13       | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 13       | 0.48          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 13       | 0.48          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 13       | 0.48          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 13       | 0.48          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 13       | 0.48          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 13       | 0.48          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 13       | 0.48          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 13       | 0.48          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 5        | 0.48          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG12 | 5        | 0.48          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG13 | 5        | 0.48          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 6        | 0.48          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG12 | 6        | 0.48          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG13 | 6        | 0.48          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG11 | 7        | 0.48          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG12 | 7        | 0.48          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG13 | 7        | 0.48          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21  | 14       | 0.48          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG22  | 14       | 0.48          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG23  | 14       | 0.48          |
| (1,1241) | 1:120:A:LYS:HE2  | 1:53:A:VAL:HG11  | 11       | 0.48          |
| (1,1241) | 1:120:A:LYS:HE2  | 1:53:A:VAL:HG12  | 11       | 0.48          |
| (1,1241) | 1:120:A:LYS:HE2  | 1:53:A:VAL:HG13  | 11       | 0.48          |
| (1,1241) | 1:120:A:LYS:HE3  | 1:53:A:VAL:HG11  | 11       | 0.48          |
| (1,1241) | 1:120:A:LYS:HE3  | 1:53:A:VAL:HG12  | 11       | 0.48          |
| (1,1241) | 1:120:A:LYS:HE3  | 1:53:A:VAL:HG13  | 11       | 0.48          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11  | 5        | 0.48          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12  | 5        | 0.48          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13  | 5        | 0.48          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11  | 5        | 0.48          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12  | 5        | 0.48          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13  | 5        | 0.48          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11  | 17       | 0.48          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12  | 17       | 0.48          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13  | 17       | 0.48          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11  | 17       | 0.48          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12  | 17       | 0.48          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13  | 17       | 0.48          |
| (1,915)  | 1:87:A:PRO:HD2   | 1:37:A:LEU:HD11  | 17       | 0.48          |
| (1,915)  | 1:87:A:PRO:HD2   | 1:37:A:LEU:HD12  | 17       | 0.48          |
| (1,915)  | 1:87:A:PRO:HD2   | 1:37:A:LEU:HD13  | 17       | 0.48          |
| (1,915)  | 1:87:A:PRO:HD3   | 1:37:A:LEU:HD11  | 17       | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,915)  | 1:87:A:PRO:HD3   | 1:37:A:LEU:HD12  | 17       | 0.48          |
| (1,915)  | 1:87:A:PRO:HD3   | 1:37:A:LEU:HD13  | 17       | 0.48          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 10       | 0.48          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 10       | 0.48          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 10       | 0.48          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 10       | 0.48          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 10       | 0.48          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 10       | 0.48          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 1        | 0.48          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 1        | 0.48          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 1        | 0.48          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 5        | 0.48          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 5        | 0.48          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 5        | 0.48          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 9        | 0.48          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 9        | 0.48          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 9        | 0.48          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H     | 1        | 0.48          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H     | 1        | 0.48          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H     | 1        | 0.48          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 16       | 0.47          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 16       | 0.47          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 16       | 0.47          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 16       | 0.47          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 16       | 0.47          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 16       | 0.47          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 16       | 0.47          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 16       | 0.47          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 16       | 0.47          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 16       | 0.47          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 16       | 0.47          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 16       | 0.47          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 8        | 0.47          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 8        | 0.47          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 8        | 0.47          |
| (1,1756) | 1:86:A:LEU:HD11  | 1:84:A:VAL:HA    | 2        | 0.47          |
| (1,1756) | 1:86:A:LEU:HD12  | 1:84:A:VAL:HA    | 2        | 0.47          |
| (1,1756) | 1:86:A:LEU:HD13  | 1:84:A:VAL:HA    | 2        | 0.47          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11  | 2        | 0.47          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12  | 2        | 0.47          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13  | 2        | 0.47          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11  | 2        | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12  | 2        | 0.47          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13  | 2        | 0.47          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA    | 8        | 0.47          |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA    | 8        | 0.47          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA    | 8        | 0.47          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 4        | 0.47          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 4        | 0.47          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 4        | 0.47          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 2        | 0.47          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 2        | 0.47          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 2        | 0.47          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 2        | 0.47          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 2        | 0.47          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 2        | 0.47          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2   | 16       | 0.47          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3   | 16       | 0.47          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2   | 16       | 0.47          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3   | 16       | 0.47          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2   | 16       | 0.47          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3   | 16       | 0.47          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2   | 20       | 0.47          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3   | 20       | 0.47          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2   | 20       | 0.47          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3   | 20       | 0.47          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2   | 20       | 0.47          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3   | 20       | 0.47          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 4        | 0.46          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 4        | 0.46          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 4        | 0.46          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 4        | 0.46          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 4        | 0.46          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 4        | 0.46          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 4        | 0.46          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 4        | 0.46          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 4        | 0.46          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 4        | 0.46          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 4        | 0.46          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 4        | 0.46          |
| (1,3520) | 1:111:A:VAL:HG11 | 1:110:A:GLU:H    | 10       | 0.46          |
| (1,3520) | 1:111:A:VAL:HG12 | 1:110:A:GLU:H    | 10       | 0.46          |
| (1,3520) | 1:111:A:VAL:HG13 | 1:110:A:GLU:H    | 10       | 0.46          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 2        | 0.46          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2566) | 1:119:A:VAL:HA  | 1:123:A:VAL:HG12 | 2        | 0.46          |
| (1,2566) | 1:119:A:VAL:HA  | 1:123:A:VAL:HG13 | 2        | 0.46          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG11 | 10       | 0.46          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG12 | 10       | 0.46          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG13 | 10       | 0.46          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG11 | 15       | 0.46          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG12 | 15       | 0.46          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG13 | 15       | 0.46          |
| (1,1756) | 1:86:A:LEU:HD11 | 1:84:A:VAL:HA    | 7        | 0.46          |
| (1,1756) | 1:86:A:LEU:HD12 | 1:84:A:VAL:HA    | 7        | 0.46          |
| (1,1756) | 1:86:A:LEU:HD13 | 1:84:A:VAL:HA    | 7        | 0.46          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG21  | 11       | 0.46          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG22  | 11       | 0.46          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG23  | 11       | 0.46          |
| (1,267)  | 1:76:A:VAL:HA   | 1:4:A:VAL:HG21   | 6        | 0.46          |
| (1,267)  | 1:76:A:VAL:HA   | 1:4:A:VAL:HG22   | 6        | 0.46          |
| (1,267)  | 1:76:A:VAL:HA   | 1:4:A:VAL:HG23   | 6        | 0.46          |
| (1,2565) | 1:18:A:ALA:HA   | 1:123:A:VAL:HG11 | 2        | 0.45          |
| (1,2565) | 1:18:A:ALA:HA   | 1:123:A:VAL:HG12 | 2        | 0.45          |
| (1,2565) | 1:18:A:ALA:HA   | 1:123:A:VAL:HG13 | 2        | 0.45          |
| (1,2434) | 1:79:A:LEU:HD21 | 1:119:A:VAL:HG21 | 16       | 0.45          |
| (1,2434) | 1:79:A:LEU:HD21 | 1:119:A:VAL:HG22 | 16       | 0.45          |
| (1,2434) | 1:79:A:LEU:HD21 | 1:119:A:VAL:HG23 | 16       | 0.45          |
| (1,2434) | 1:79:A:LEU:HD22 | 1:119:A:VAL:HG21 | 16       | 0.45          |
| (1,2434) | 1:79:A:LEU:HD22 | 1:119:A:VAL:HG22 | 16       | 0.45          |
| (1,2434) | 1:79:A:LEU:HD22 | 1:119:A:VAL:HG23 | 16       | 0.45          |
| (1,2434) | 1:79:A:LEU:HD23 | 1:119:A:VAL:HG21 | 16       | 0.45          |
| (1,2434) | 1:79:A:LEU:HD23 | 1:119:A:VAL:HG22 | 16       | 0.45          |
| (1,2434) | 1:79:A:LEU:HD23 | 1:119:A:VAL:HG23 | 16       | 0.45          |
| (1,1776) | 1:37:A:LEU:HD11 | 1:86:A:LEU:HA    | 11       | 0.45          |
| (1,1776) | 1:37:A:LEU:HD12 | 1:86:A:LEU:HA    | 11       | 0.45          |
| (1,1776) | 1:37:A:LEU:HD13 | 1:86:A:LEU:HA    | 11       | 0.45          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG11  | 2        | 0.45          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG12  | 2        | 0.45          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG13  | 2        | 0.45          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG11  | 2        | 0.45          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG12  | 2        | 0.45          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG13  | 2        | 0.45          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD11  | 11       | 0.45          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD12  | 11       | 0.45          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD13  | 11       | 0.45          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG11  | 17       | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG12  | 17       | 0.45          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG13  | 17       | 0.45          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA    | 2        | 0.45          |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA    | 2        | 0.45          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA    | 2        | 0.45          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11   | 7        | 0.45          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12   | 7        | 0.45          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13   | 7        | 0.45          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11   | 7        | 0.45          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12   | 7        | 0.45          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13   | 7        | 0.45          |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD21  | 11       | 0.44          |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD22  | 11       | 0.44          |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD21  | 11       | 0.44          |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD22  | 11       | 0.44          |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD21  | 11       | 0.44          |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD22  | 11       | 0.44          |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD21  | 11       | 0.44          |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD22  | 11       | 0.44          |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD21  | 11       | 0.44          |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD22  | 11       | 0.44          |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD21  | 11       | 0.44          |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD22  | 11       | 0.44          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 5        | 0.44          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 5        | 0.44          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 5        | 0.44          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 3        | 0.44          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 3        | 0.44          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 3        | 0.44          |
| (1,2357) | 1:119:A:VAL:HG11 | 1:116:A:ARG:HG2  | 19       | 0.44          |
| (1,2357) | 1:119:A:VAL:HG11 | 1:116:A:ARG:HG3  | 19       | 0.44          |
| (1,2357) | 1:119:A:VAL:HG12 | 1:116:A:ARG:HG2  | 19       | 0.44          |
| (1,2357) | 1:119:A:VAL:HG12 | 1:116:A:ARG:HG3  | 19       | 0.44          |
| (1,2357) | 1:119:A:VAL:HG13 | 1:116:A:ARG:HG2  | 19       | 0.44          |
| (1,2357) | 1:119:A:VAL:HG13 | 1:116:A:ARG:HG3  | 19       | 0.44          |
| (1,1798) | 1:76:A:VAL:HG11  | 1:86:A:LEU:HD11  | 17       | 0.44          |
| (1,1798) | 1:76:A:VAL:HG11  | 1:86:A:LEU:HD12  | 17       | 0.44          |
| (1,1798) | 1:76:A:VAL:HG11  | 1:86:A:LEU:HD13  | 17       | 0.44          |
| (1,1798) | 1:76:A:VAL:HG12  | 1:86:A:LEU:HD11  | 17       | 0.44          |
| (1,1798) | 1:76:A:VAL:HG12  | 1:86:A:LEU:HD12  | 17       | 0.44          |
| (1,1798) | 1:76:A:VAL:HG12  | 1:86:A:LEU:HD13  | 17       | 0.44          |
| (1,1798) | 1:76:A:VAL:HG13  | 1:86:A:LEU:HD11  | 17       | 0.44          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1798) | 1:76:A:VAL:HG13 | 1:86:A:LEU:HD12 | 17       | 0.44          |
| (1,1798) | 1:76:A:VAL:HG13 | 1:86:A:LEU:HD13 | 17       | 0.44          |
| (1,1776) | 1:37:A:LEU:HD11 | 1:86:A:LEU:HA   | 14       | 0.44          |
| (1,1776) | 1:37:A:LEU:HD12 | 1:86:A:LEU:HA   | 14       | 0.44          |
| (1,1776) | 1:37:A:LEU:HD13 | 1:86:A:LEU:HA   | 14       | 0.44          |
| (1,1776) | 1:37:A:LEU:HD11 | 1:86:A:LEU:HA   | 15       | 0.44          |
| (1,1776) | 1:37:A:LEU:HD12 | 1:86:A:LEU:HA   | 15       | 0.44          |
| (1,1776) | 1:37:A:LEU:HD13 | 1:86:A:LEU:HA   | 15       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB2  | 1:53:A:VAL:HG21 | 14       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB2  | 1:53:A:VAL:HG22 | 14       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB2  | 1:53:A:VAL:HG23 | 14       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB3  | 1:53:A:VAL:HG21 | 14       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB3  | 1:53:A:VAL:HG22 | 14       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB3  | 1:53:A:VAL:HG23 | 14       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB2  | 1:53:A:VAL:HG21 | 14       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB2  | 1:53:A:VAL:HG22 | 14       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB2  | 1:53:A:VAL:HG23 | 14       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB3  | 1:53:A:VAL:HG21 | 14       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB3  | 1:53:A:VAL:HG22 | 14       | 0.44          |
| (1,1250) | 1:52:A:GLU:HB3  | 1:53:A:VAL:HG23 | 14       | 0.44          |
| (1,1248) | 1:53:A:VAL:H    | 1:53:A:VAL:HG21 | 13       | 0.44          |
| (1,1248) | 1:53:A:VAL:H    | 1:53:A:VAL:HG22 | 13       | 0.44          |
| (1,1248) | 1:53:A:VAL:H    | 1:53:A:VAL:HG23 | 13       | 0.44          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD11 | 14       | 0.44          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD12 | 14       | 0.44          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD13 | 14       | 0.44          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD11 | 15       | 0.44          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD12 | 15       | 0.44          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD13 | 15       | 0.44          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG21 | 15       | 0.44          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG22 | 15       | 0.44          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG23 | 15       | 0.44          |
| (1,805)  | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG11 | 8        | 0.44          |
| (1,805)  | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG12 | 8        | 0.44          |
| (1,805)  | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG13 | 8        | 0.44          |
| (1,805)  | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG11 | 8        | 0.44          |
| (1,805)  | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG12 | 8        | 0.44          |
| (1,805)  | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG13 | 8        | 0.44          |
| (1,313)  | 1:5:A:MET:HG2   | 1:7:A:VAL:HG11  | 10       | 0.44          |
| (1,313)  | 1:5:A:MET:HG2   | 1:7:A:VAL:HG12  | 10       | 0.44          |
| (1,313)  | 1:5:A:MET:HG2   | 1:7:A:VAL:HG13  | 10       | 0.44          |
| (1,313)  | 1:5:A:MET:HG3   | 1:7:A:VAL:HG11  | 10       | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12   | 10       | 0.44          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13   | 10       | 0.44          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11   | 15       | 0.44          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12   | 15       | 0.44          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13   | 15       | 0.44          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11   | 15       | 0.44          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12   | 15       | 0.44          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13   | 15       | 0.44          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 8        | 0.44          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 8        | 0.44          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 8        | 0.44          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 8        | 0.44          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 8        | 0.44          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 8        | 0.44          |
| (1,60)   | 1:79:A:LEU:HD11  | 1:78:A:SER:H     | 5        | 0.44          |
| (1,60)   | 1:79:A:LEU:HD12  | 1:78:A:SER:H     | 5        | 0.44          |
| (1,60)   | 1:79:A:LEU:HD13  | 1:78:A:SER:H     | 5        | 0.44          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 7        | 0.43          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 7        | 0.43          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 7        | 0.43          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 7        | 0.43          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 7        | 0.43          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 7        | 0.43          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 7        | 0.43          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 7        | 0.43          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 7        | 0.43          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 7        | 0.43          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 7        | 0.43          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 7        | 0.43          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 3        | 0.43          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 3        | 0.43          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 3        | 0.43          |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA    | 4        | 0.43          |
| (1,1776) | 1:37:A:LEU:HD12  | 1:86:A:LEU:HA    | 4        | 0.43          |
| (1,1776) | 1:37:A:LEU:HD13  | 1:86:A:LEU:HA    | 4        | 0.43          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD11  | 4        | 0.43          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12  | 4        | 0.43          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13  | 4        | 0.43          |
| (1,405)  | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB   | 12       | 0.43          |
| (1,405)  | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB   | 12       | 0.43          |
| (1,405)  | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB   | 12       | 0.43          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG11   | 12       | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG12   | 12       | 0.43          |
| (1,313)  | 1:5:A:MET:HG2    | 1:7:A:VAL:HG13   | 12       | 0.43          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG11   | 12       | 0.43          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG12   | 12       | 0.43          |
| (1,313)  | 1:5:A:MET:HG3    | 1:7:A:VAL:HG13   | 12       | 0.43          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG11   | 19       | 0.43          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG12   | 19       | 0.43          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG13   | 19       | 0.43          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG11   | 20       | 0.43          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG12   | 20       | 0.43          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG13   | 20       | 0.43          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE2  | 17       | 0.42          |
| (1,2708) | 1:126:A:LEU:HD11 | 1:129:A:LYS:HE3  | 17       | 0.42          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE2  | 17       | 0.42          |
| (1,2708) | 1:126:A:LEU:HD12 | 1:129:A:LYS:HE3  | 17       | 0.42          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE2  | 17       | 0.42          |
| (1,2708) | 1:126:A:LEU:HD13 | 1:129:A:LYS:HE3  | 17       | 0.42          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD11 | 17       | 0.42          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD12 | 17       | 0.42          |
| (1,2640) | 1:129:A:LYS:HE2  | 1:126:A:LEU:HD13 | 17       | 0.42          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD11 | 17       | 0.42          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD12 | 17       | 0.42          |
| (1,2640) | 1:129:A:LYS:HE3  | 1:126:A:LEU:HD13 | 17       | 0.42          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 13       | 0.42          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 13       | 0.42          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 13       | 0.42          |
| (1,1248) | 1:53:A:VAL:H     | 1:53:A:VAL:HG21  | 14       | 0.42          |
| (1,1248) | 1:53:A:VAL:H     | 1:53:A:VAL:HG22  | 14       | 0.42          |
| (1,1248) | 1:53:A:VAL:H     | 1:53:A:VAL:HG23  | 14       | 0.42          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11  | 6        | 0.42          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12  | 6        | 0.42          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13  | 6        | 0.42          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11  | 6        | 0.42          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12  | 6        | 0.42          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13  | 6        | 0.42          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11  | 19       | 0.42          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12  | 19       | 0.42          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13  | 19       | 0.42          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11  | 19       | 0.42          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12  | 19       | 0.42          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13  | 19       | 0.42          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11  | 6        | 0.42          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,805) | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12 | 6        | 0.42          |
| (1,805) | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13 | 6        | 0.42          |
| (1,805) | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11 | 6        | 0.42          |
| (1,805) | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12 | 6        | 0.42          |
| (1,805) | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13 | 6        | 0.42          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11 | 17       | 0.42          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12 | 17       | 0.42          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13 | 17       | 0.42          |
| (1,648) | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA   | 17       | 0.42          |
| (1,648) | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA   | 17       | 0.42          |
| (1,648) | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA   | 17       | 0.42          |
| (1,569) | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB1  | 7        | 0.42          |
| (1,569) | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB2  | 7        | 0.42          |
| (1,569) | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB3  | 7        | 0.42          |
| (1,569) | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB1  | 7        | 0.42          |
| (1,569) | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB2  | 7        | 0.42          |
| (1,569) | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB3  | 7        | 0.42          |
| (1,569) | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB1  | 7        | 0.42          |
| (1,569) | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB2  | 7        | 0.42          |
| (1,569) | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB3  | 7        | 0.42          |
| (1,480) | 1:119:A:VAL:HG11 | 1:17:A:MET:HG2  | 16       | 0.42          |
| (1,480) | 1:119:A:VAL:HG11 | 1:17:A:MET:HG3  | 16       | 0.42          |
| (1,480) | 1:119:A:VAL:HG12 | 1:17:A:MET:HG2  | 16       | 0.42          |
| (1,480) | 1:119:A:VAL:HG12 | 1:17:A:MET:HG3  | 16       | 0.42          |
| (1,480) | 1:119:A:VAL:HG13 | 1:17:A:MET:HG2  | 16       | 0.42          |
| (1,480) | 1:119:A:VAL:HG13 | 1:17:A:MET:HG3  | 16       | 0.42          |
| (1,405) | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB  | 10       | 0.42          |
| (1,405) | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB  | 10       | 0.42          |
| (1,405) | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB  | 10       | 0.42          |
| (1,278) | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG21  | 6        | 0.42          |
| (1,278) | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG22  | 6        | 0.42          |
| (1,278) | 1:32:A:VAL:HG21  | 1:4:A:VAL:HG23  | 6        | 0.42          |
| (1,278) | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG21  | 6        | 0.42          |
| (1,278) | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG22  | 6        | 0.42          |
| (1,278) | 1:32:A:VAL:HG22  | 1:4:A:VAL:HG23  | 6        | 0.42          |
| (1,278) | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG21  | 6        | 0.42          |
| (1,278) | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG22  | 6        | 0.42          |
| (1,278) | 1:32:A:VAL:HG23  | 1:4:A:VAL:HG23  | 6        | 0.42          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG11  | 8        | 0.42          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG12  | 8        | 0.42          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG13  | 8        | 0.42          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG11  | 11       | 0.42          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,251)  | 1:4:A:VAL:H     | 1:4:A:VAL:HG12   | 11       | 0.42          |
| (1,251)  | 1:4:A:VAL:H     | 1:4:A:VAL:HG13   | 11       | 0.42          |
| (1,251)  | 1:4:A:VAL:H     | 1:4:A:VAL:HG11   | 14       | 0.42          |
| (1,251)  | 1:4:A:VAL:H     | 1:4:A:VAL:HG12   | 14       | 0.42          |
| (1,251)  | 1:4:A:VAL:H     | 1:4:A:VAL:HG13   | 14       | 0.42          |
| (1,91)   | 1:32:A:VAL:HG11 | 1:6:A:PHE:HD1    | 6        | 0.42          |
| (1,91)   | 1:32:A:VAL:HG11 | 1:6:A:PHE:HD2    | 6        | 0.42          |
| (1,91)   | 1:32:A:VAL:HG12 | 1:6:A:PHE:HD1    | 6        | 0.42          |
| (1,91)   | 1:32:A:VAL:HG12 | 1:6:A:PHE:HD2    | 6        | 0.42          |
| (1,91)   | 1:32:A:VAL:HG13 | 1:6:A:PHE:HD1    | 6        | 0.42          |
| (1,91)   | 1:32:A:VAL:HG13 | 1:6:A:PHE:HD2    | 6        | 0.42          |
| (1,60)   | 1:79:A:LEU:HD11 | 1:78:A:SER:H     | 7        | 0.42          |
| (1,60)   | 1:79:A:LEU:HD12 | 1:78:A:SER:H     | 7        | 0.42          |
| (1,60)   | 1:79:A:LEU:HD13 | 1:78:A:SER:H     | 7        | 0.42          |
| (1,2566) | 1:119:A:VAL:HA  | 1:123:A:VAL:HG11 | 1        | 0.41          |
| (1,2566) | 1:119:A:VAL:HA  | 1:123:A:VAL:HG12 | 1        | 0.41          |
| (1,2566) | 1:119:A:VAL:HA  | 1:123:A:VAL:HG13 | 1        | 0.41          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD11  | 7        | 0.41          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD12  | 7        | 0.41          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD13  | 7        | 0.41          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG21 | 13       | 0.41          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG22 | 13       | 0.41          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG23 | 13       | 0.41          |
| (1,814)  | 1:25:A:LEU:HB3  | 1:123:A:VAL:HG21 | 13       | 0.41          |
| (1,814)  | 1:25:A:LEU:HB3  | 1:123:A:VAL:HG22 | 13       | 0.41          |
| (1,814)  | 1:25:A:LEU:HB3  | 1:123:A:VAL:HG23 | 13       | 0.41          |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG21  | 8        | 0.41          |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG22  | 8        | 0.41          |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG23  | 8        | 0.41          |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG21  | 8        | 0.41          |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG22  | 8        | 0.41          |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG23  | 8        | 0.41          |
| (1,812)  | 1:4:A:VAL:HG23  | 1:32:A:VAL:HG21  | 8        | 0.41          |
| (1,812)  | 1:4:A:VAL:HG23  | 1:32:A:VAL:HG22  | 8        | 0.41          |
| (1,812)  | 1:4:A:VAL:HG23  | 1:32:A:VAL:HG23  | 8        | 0.41          |
| (1,805)  | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG11  | 12       | 0.41          |
| (1,805)  | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG12  | 12       | 0.41          |
| (1,805)  | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG13  | 12       | 0.41          |
| (1,805)  | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG11  | 12       | 0.41          |
| (1,805)  | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG12  | 12       | 0.41          |
| (1,805)  | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG13  | 12       | 0.41          |
| (1,668)  | 1:25:A:LEU:HA   | 1:25:A:LEU:HD11  | 10       | 0.41          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12 | 10       | 0.41          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13 | 10       | 0.41          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11 | 11       | 0.41          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12 | 11       | 0.41          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13 | 11       | 0.41          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11 | 15       | 0.41          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12 | 15       | 0.41          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13 | 15       | 0.41          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11 | 19       | 0.41          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12 | 19       | 0.41          |
| (1,668) | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13 | 19       | 0.41          |
| (1,648) | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA   | 10       | 0.41          |
| (1,648) | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA   | 10       | 0.41          |
| (1,648) | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA   | 10       | 0.41          |
| (1,648) | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA   | 11       | 0.41          |
| (1,648) | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA   | 11       | 0.41          |
| (1,648) | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA   | 11       | 0.41          |
| (1,648) | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA   | 15       | 0.41          |
| (1,648) | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA   | 15       | 0.41          |
| (1,648) | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA   | 15       | 0.41          |
| (1,648) | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA   | 19       | 0.41          |
| (1,648) | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA   | 19       | 0.41          |
| (1,648) | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA   | 19       | 0.41          |
| (1,569) | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB1  | 9        | 0.41          |
| (1,569) | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB2  | 9        | 0.41          |
| (1,569) | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB3  | 9        | 0.41          |
| (1,569) | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB1  | 9        | 0.41          |
| (1,569) | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB2  | 9        | 0.41          |
| (1,569) | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB3  | 9        | 0.41          |
| (1,569) | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB1  | 9        | 0.41          |
| (1,569) | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB2  | 9        | 0.41          |
| (1,569) | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB3  | 9        | 0.41          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG11  | 3        | 0.41          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG12  | 3        | 0.41          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG13  | 3        | 0.41          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG11  | 4        | 0.41          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG12  | 4        | 0.41          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG13  | 4        | 0.41          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG11  | 5        | 0.41          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG12  | 5        | 0.41          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG13  | 5        | 0.41          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG11  | 12       | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG12   | 12       | 0.41          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG13   | 12       | 0.41          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG11   | 16       | 0.41          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG12   | 16       | 0.41          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG13   | 16       | 0.41          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 12       | 0.41          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 12       | 0.41          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 12       | 0.41          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 12       | 0.41          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 12       | 0.41          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 12       | 0.41          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA    | 16       | 0.41          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA    | 16       | 0.41          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA    | 16       | 0.41          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD11  | 14       | 0.41          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD12  | 14       | 0.41          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD13  | 14       | 0.41          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 6        | 0.4           |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 6        | 0.4           |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 6        | 0.4           |
| (1,3324) | 1:4:A:VAL:HG21   | 1:75:A:VAL:H     | 6        | 0.4           |
| (1,3324) | 1:4:A:VAL:HG22   | 1:75:A:VAL:H     | 6        | 0.4           |
| (1,3324) | 1:4:A:VAL:HG23   | 1:75:A:VAL:H     | 6        | 0.4           |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 4        | 0.4           |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG12 | 4        | 0.4           |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG13 | 4        | 0.4           |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 12       | 0.4           |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG12 | 12       | 0.4           |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG13 | 12       | 0.4           |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 6        | 0.4           |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 6        | 0.4           |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 6        | 0.4           |
| (1,2357) | 1:119:A:VAL:HG11 | 1:116:A:ARG:HG2  | 1        | 0.4           |
| (1,2357) | 1:119:A:VAL:HG11 | 1:116:A:ARG:HG3  | 1        | 0.4           |
| (1,2357) | 1:119:A:VAL:HG12 | 1:116:A:ARG:HG2  | 1        | 0.4           |
| (1,2357) | 1:119:A:VAL:HG12 | 1:116:A:ARG:HG3  | 1        | 0.4           |
| (1,2357) | 1:119:A:VAL:HG13 | 1:116:A:ARG:HG2  | 1        | 0.4           |
| (1,2357) | 1:119:A:VAL:HG13 | 1:116:A:ARG:HG3  | 1        | 0.4           |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG21 | 16       | 0.4           |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG22 | 16       | 0.4           |
| (1,2247) | 1:102:A:GLU:HB2  | 1:111:A:VAL:HG23 | 16       | 0.4           |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG21 | 16       | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG22 | 16       | 0.4           |
| (1,2247) | 1:102:A:GLU:HB3  | 1:111:A:VAL:HG23 | 16       | 0.4           |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA   | 10       | 0.4           |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA   | 10       | 0.4           |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA   | 10       | 0.4           |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD11  | 10       | 0.4           |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD12  | 10       | 0.4           |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD13  | 10       | 0.4           |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD11  | 10       | 0.4           |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD12  | 10       | 0.4           |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD13  | 10       | 0.4           |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD11  | 10       | 0.4           |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD12  | 10       | 0.4           |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD13  | 10       | 0.4           |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 8        | 0.4           |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 8        | 0.4           |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 8        | 0.4           |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 9        | 0.4           |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 9        | 0.4           |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 9        | 0.4           |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 13       | 0.4           |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 13       | 0.4           |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 13       | 0.4           |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG21  | 18       | 0.4           |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG22  | 18       | 0.4           |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG23  | 18       | 0.4           |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11  | 19       | 0.4           |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG12  | 19       | 0.4           |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG13  | 19       | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 1        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12  | 1        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13  | 1        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 2        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12  | 2        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13  | 2        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 4        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12  | 4        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13  | 4        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 9        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12  | 9        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13  | 9        | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 14       | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12  | 14       | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13  | 14       | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 16       | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12  | 16       | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13  | 16       | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 20       | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12  | 20       | 0.4           |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13  | 20       | 0.4           |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA    | 1        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA    | 1        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA    | 1        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA    | 2        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA    | 2        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA    | 2        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA    | 4        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA    | 4        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA    | 4        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA    | 9        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA    | 9        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA    | 9        | 0.4           |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA    | 14       | 0.4           |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA    | 14       | 0.4           |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA    | 14       | 0.4           |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA    | 16       | 0.4           |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA    | 16       | 0.4           |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA    | 16       | 0.4           |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA    | 20       | 0.4           |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA    | 20       | 0.4           |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA    | 20       | 0.4           |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA    | 6        | 0.4           |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA    | 6        | 0.4           |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA    | 6        | 0.4           |
| (1,273)  | 1:75:A:VAL:H     | 1:4:A:VAL:HG21   | 6        | 0.4           |
| (1,273)  | 1:75:A:VAL:H     | 1:4:A:VAL:HG22   | 6        | 0.4           |
| (1,273)  | 1:75:A:VAL:H     | 1:4:A:VAL:HG23   | 6        | 0.4           |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG11   | 2        | 0.4           |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG12   | 2        | 0.4           |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG13   | 2        | 0.4           |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG11   | 15       | 0.4           |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG12   | 15       | 0.4           |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG13   | 15       | 0.4           |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 15       | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 15       | 0.39          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 15       | 0.39          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 19       | 0.39          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 19       | 0.39          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 19       | 0.39          |
| (1,2357) | 1:119:A:VAL:HG11 | 1:116:A:ARG:HG2  | 20       | 0.39          |
| (1,2357) | 1:119:A:VAL:HG11 | 1:116:A:ARG:HG3  | 20       | 0.39          |
| (1,2357) | 1:119:A:VAL:HG12 | 1:116:A:ARG:HG2  | 20       | 0.39          |
| (1,2357) | 1:119:A:VAL:HG12 | 1:116:A:ARG:HG3  | 20       | 0.39          |
| (1,2357) | 1:119:A:VAL:HG13 | 1:116:A:ARG:HG2  | 20       | 0.39          |
| (1,2357) | 1:119:A:VAL:HG13 | 1:116:A:ARG:HG3  | 20       | 0.39          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11  | 5        | 0.39          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12  | 5        | 0.39          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13  | 5        | 0.39          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21  | 10       | 0.39          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG22  | 10       | 0.39          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG23  | 10       | 0.39          |
| (1,1248) | 1:53:A:VAL:H     | 1:53:A:VAL:HG21  | 9        | 0.39          |
| (1,1248) | 1:53:A:VAL:H     | 1:53:A:VAL:HG22  | 9        | 0.39          |
| (1,1248) | 1:53:A:VAL:H     | 1:53:A:VAL:HG23  | 9        | 0.39          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 15       | 0.39          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 15       | 0.39          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 15       | 0.39          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 17       | 0.39          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 17       | 0.39          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 17       | 0.39          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11  | 7        | 0.39          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12  | 7        | 0.39          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13  | 7        | 0.39          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11  | 7        | 0.39          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12  | 7        | 0.39          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13  | 7        | 0.39          |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 6        | 0.39          |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12  | 6        | 0.39          |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13  | 6        | 0.39          |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 7        | 0.39          |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12  | 7        | 0.39          |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13  | 7        | 0.39          |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 12       | 0.39          |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12  | 12       | 0.39          |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13  | 12       | 0.39          |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD11  | 13       | 0.39          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD12 | 13       | 0.39          |
| (1,668)  | 1:25:A:LEU:HA    | 1:25:A:LEU:HD13 | 13       | 0.39          |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA   | 6        | 0.39          |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA   | 6        | 0.39          |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA   | 6        | 0.39          |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA   | 7        | 0.39          |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA   | 7        | 0.39          |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA   | 7        | 0.39          |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA   | 12       | 0.39          |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA   | 12       | 0.39          |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA   | 12       | 0.39          |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA   | 13       | 0.39          |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA   | 13       | 0.39          |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA   | 13       | 0.39          |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG2  | 19       | 0.39          |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG3  | 19       | 0.39          |
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG2  | 19       | 0.39          |
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG3  | 19       | 0.39          |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG2  | 19       | 0.39          |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG3  | 19       | 0.39          |
| (1,405)  | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB  | 15       | 0.39          |
| (1,405)  | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB  | 15       | 0.39          |
| (1,405)  | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB  | 15       | 0.39          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG11  | 1        | 0.39          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG12  | 1        | 0.39          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG13  | 1        | 0.39          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG11  | 18       | 0.39          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG12  | 18       | 0.39          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG13  | 18       | 0.39          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ    | 14       | 0.39          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ    | 14       | 0.39          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ    | 14       | 0.39          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1   | 7        | 0.39          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2   | 7        | 0.39          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1   | 7        | 0.39          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2   | 7        | 0.39          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1   | 7        | 0.39          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2   | 7        | 0.39          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA   | 6        | 0.39          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA   | 6        | 0.39          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA   | 6        | 0.39          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H   | 8        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 8        | 0.38          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 8        | 0.38          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG11 | 14       | 0.38          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG12 | 14       | 0.38          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG13 | 14       | 0.38          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA   | 17       | 0.38          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA   | 17       | 0.38          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA   | 17       | 0.38          |
| (1,1247) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG21  | 3        | 0.38          |
| (1,1247) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG22  | 3        | 0.38          |
| (1,1247) | 1:21:A:PHE:HD1   | 1:53:A:VAL:HG23  | 3        | 0.38          |
| (1,1247) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG21  | 3        | 0.38          |
| (1,1247) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG22  | 3        | 0.38          |
| (1,1247) | 1:21:A:PHE:HD2   | 1:53:A:VAL:HG23  | 3        | 0.38          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD21  | 4        | 0.38          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD22  | 4        | 0.38          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD23  | 4        | 0.38          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD21  | 4        | 0.38          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD22  | 4        | 0.38          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD23  | 4        | 0.38          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD21  | 14       | 0.38          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD22  | 14       | 0.38          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD23  | 14       | 0.38          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD21  | 14       | 0.38          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD22  | 14       | 0.38          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD23  | 14       | 0.38          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD21  | 16       | 0.38          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD22  | 16       | 0.38          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD23  | 16       | 0.38          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD21  | 16       | 0.38          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD22  | 16       | 0.38          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD23  | 16       | 0.38          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 2        | 0.38          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 2        | 0.38          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 2        | 0.38          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 4        | 0.38          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 4        | 0.38          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 4        | 0.38          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 14       | 0.38          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 14       | 0.38          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 14       | 0.38          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG21  | 2        | 0.38          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,821) | 1:33:A:THR:H    | 1:32:A:VAL:HG22 | 2        | 0.38          |
| (1,821) | 1:33:A:THR:H    | 1:32:A:VAL:HG23 | 2        | 0.38          |
| (1,813) | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG21 | 5        | 0.38          |
| (1,813) | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG22 | 5        | 0.38          |
| (1,813) | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG23 | 5        | 0.38          |
| (1,813) | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG21 | 5        | 0.38          |
| (1,813) | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG22 | 5        | 0.38          |
| (1,813) | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG23 | 5        | 0.38          |
| (1,810) | 1:33:A:THR:H    | 1:32:A:VAL:HG11 | 20       | 0.38          |
| (1,810) | 1:33:A:THR:H    | 1:32:A:VAL:HG12 | 20       | 0.38          |
| (1,810) | 1:33:A:THR:H    | 1:32:A:VAL:HG13 | 20       | 0.38          |
| (1,805) | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG11 | 1        | 0.38          |
| (1,805) | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG12 | 1        | 0.38          |
| (1,805) | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG13 | 1        | 0.38          |
| (1,805) | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG11 | 1        | 0.38          |
| (1,805) | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG12 | 1        | 0.38          |
| (1,805) | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG13 | 1        | 0.38          |
| (1,805) | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG11 | 18       | 0.38          |
| (1,805) | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG12 | 18       | 0.38          |
| (1,805) | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG13 | 18       | 0.38          |
| (1,805) | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG11 | 18       | 0.38          |
| (1,805) | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG12 | 18       | 0.38          |
| (1,805) | 1:6:A:PHE:HD2   | 1:32:A:VAL:HG13 | 18       | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD11 | 3        | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD12 | 3        | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD13 | 3        | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD11 | 5        | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD12 | 5        | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD13 | 5        | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD11 | 8        | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD12 | 8        | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD13 | 8        | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD11 | 18       | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD12 | 18       | 0.38          |
| (1,668) | 1:25:A:LEU:HA   | 1:25:A:LEU:HD13 | 18       | 0.38          |
| (1,648) | 1:25:A:LEU:HD11 | 1:25:A:LEU:HA   | 3        | 0.38          |
| (1,648) | 1:25:A:LEU:HD12 | 1:25:A:LEU:HA   | 3        | 0.38          |
| (1,648) | 1:25:A:LEU:HD13 | 1:25:A:LEU:HA   | 3        | 0.38          |
| (1,648) | 1:25:A:LEU:HD11 | 1:25:A:LEU:HA   | 5        | 0.38          |
| (1,648) | 1:25:A:LEU:HD12 | 1:25:A:LEU:HA   | 5        | 0.38          |
| (1,648) | 1:25:A:LEU:HD13 | 1:25:A:LEU:HA   | 5        | 0.38          |
| (1,648) | 1:25:A:LEU:HD11 | 1:25:A:LEU:HA   | 8        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA    | 8        | 0.38          |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA    | 8        | 0.38          |
| (1,648)  | 1:25:A:LEU:HD11  | 1:25:A:LEU:HA    | 18       | 0.38          |
| (1,648)  | 1:25:A:LEU:HD12  | 1:25:A:LEU:HA    | 18       | 0.38          |
| (1,648)  | 1:25:A:LEU:HD13  | 1:25:A:LEU:HA    | 18       | 0.38          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG11   | 10       | 0.38          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG12   | 10       | 0.38          |
| (1,251)  | 1:4:A:VAL:H      | 1:4:A:VAL:HG13   | 10       | 0.38          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 1        | 0.38          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 1        | 0.38          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 1        | 0.38          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 1        | 0.38          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 1        | 0.38          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 1        | 0.38          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 18       | 0.38          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 18       | 0.38          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 18       | 0.38          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 18       | 0.38          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 18       | 0.38          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 18       | 0.38          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 11       | 0.37          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 11       | 0.37          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 11       | 0.37          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 20       | 0.37          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 20       | 0.37          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 20       | 0.37          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 20       | 0.37          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG12 | 20       | 0.37          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG13 | 20       | 0.37          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 19       | 0.37          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 19       | 0.37          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 19       | 0.37          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG11 | 18       | 0.37          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG12 | 18       | 0.37          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG13 | 18       | 0.37          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 11       | 0.37          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 11       | 0.37          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 11       | 0.37          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 14       | 0.37          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 14       | 0.37          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 14       | 0.37          |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG21 | 3        | 0.37          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2245) | 1:104:A:PRO:HB2 | 1:111:A:VAL:HG22 | 3        | 0.37          |
| (1,2245) | 1:104:A:PRO:HB2 | 1:111:A:VAL:HG23 | 3        | 0.37          |
| (1,2245) | 1:104:A:PRO:HB3 | 1:111:A:VAL:HG21 | 3        | 0.37          |
| (1,2245) | 1:104:A:PRO:HB3 | 1:111:A:VAL:HG22 | 3        | 0.37          |
| (1,2245) | 1:104:A:PRO:HB3 | 1:111:A:VAL:HG23 | 3        | 0.37          |
| (1,1776) | 1:37:A:LEU:HD11 | 1:86:A:LEU:HA    | 19       | 0.37          |
| (1,1776) | 1:37:A:LEU:HD12 | 1:86:A:LEU:HA    | 19       | 0.37          |
| (1,1776) | 1:37:A:LEU:HD13 | 1:86:A:LEU:HA    | 19       | 0.37          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG21  | 2        | 0.37          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG22  | 2        | 0.37          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG23  | 2        | 0.37          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG21  | 19       | 0.37          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG22  | 19       | 0.37          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG23  | 19       | 0.37          |
| (1,1248) | 1:53:A:VAL:H    | 1:53:A:VAL:HG21  | 11       | 0.37          |
| (1,1248) | 1:53:A:VAL:H    | 1:53:A:VAL:HG22  | 11       | 0.37          |
| (1,1248) | 1:53:A:VAL:H    | 1:53:A:VAL:HG23  | 11       | 0.37          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG11  | 16       | 0.37          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG12  | 16       | 0.37          |
| (1,1239) | 1:49:A:MET:HB2  | 1:53:A:VAL:HG13  | 16       | 0.37          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG11  | 16       | 0.37          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG12  | 16       | 0.37          |
| (1,1239) | 1:49:A:MET:HB3  | 1:53:A:VAL:HG13  | 16       | 0.37          |
| (1,921)  | 1:85:A:ASN:HB2  | 1:37:A:LEU:HD21  | 18       | 0.37          |
| (1,921)  | 1:85:A:ASN:HB2  | 1:37:A:LEU:HD22  | 18       | 0.37          |
| (1,921)  | 1:85:A:ASN:HB2  | 1:37:A:LEU:HD23  | 18       | 0.37          |
| (1,921)  | 1:85:A:ASN:HB3  | 1:37:A:LEU:HD21  | 18       | 0.37          |
| (1,921)  | 1:85:A:ASN:HB3  | 1:37:A:LEU:HD22  | 18       | 0.37          |
| (1,921)  | 1:85:A:ASN:HB3  | 1:37:A:LEU:HD23  | 18       | 0.37          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD11  | 19       | 0.37          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD12  | 19       | 0.37          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD13  | 19       | 0.37          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD11  | 3        | 0.37          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD12  | 3        | 0.37          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD13  | 3        | 0.37          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD11  | 6        | 0.37          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD12  | 6        | 0.37          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD13  | 6        | 0.37          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD11  | 12       | 0.37          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD12  | 12       | 0.37          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD13  | 12       | 0.37          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD11  | 19       | 0.37          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,916) | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12 | 19       | 0.37          |
| (1,916) | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13 | 19       | 0.37          |
| (1,916) | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11 | 20       | 0.37          |
| (1,916) | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12 | 20       | 0.37          |
| (1,916) | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13 | 20       | 0.37          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG21 | 6        | 0.37          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG22 | 6        | 0.37          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG23 | 6        | 0.37          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG21 | 8        | 0.37          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG22 | 8        | 0.37          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG23 | 8        | 0.37          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG21 | 11       | 0.37          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG22 | 11       | 0.37          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG23 | 11       | 0.37          |
| (1,805) | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11 | 11       | 0.37          |
| (1,805) | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12 | 11       | 0.37          |
| (1,805) | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13 | 11       | 0.37          |
| (1,805) | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11 | 11       | 0.37          |
| (1,805) | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12 | 11       | 0.37          |
| (1,805) | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13 | 11       | 0.37          |
| (1,805) | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11 | 16       | 0.37          |
| (1,805) | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12 | 16       | 0.37          |
| (1,805) | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13 | 16       | 0.37          |
| (1,805) | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11 | 16       | 0.37          |
| (1,805) | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12 | 16       | 0.37          |
| (1,805) | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13 | 16       | 0.37          |
| (1,483) | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA   | 19       | 0.37          |
| (1,483) | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA   | 19       | 0.37          |
| (1,483) | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA   | 19       | 0.37          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG11  | 9        | 0.37          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG12  | 9        | 0.37          |
| (1,251) | 1:4:A:VAL:H      | 1:4:A:VAL:HG13  | 9        | 0.37          |
| (1,91)  | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1   | 11       | 0.37          |
| (1,91)  | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2   | 11       | 0.37          |
| (1,91)  | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1   | 11       | 0.37          |
| (1,91)  | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2   | 11       | 0.37          |
| (1,91)  | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1   | 11       | 0.37          |
| (1,91)  | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2   | 11       | 0.37          |
| (1,91)  | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1   | 16       | 0.37          |
| (1,91)  | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2   | 16       | 0.37          |
| (1,91)  | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1   | 16       | 0.37          |
| (1,91)  | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2   | 16       | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 16       | 0.37          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 16       | 0.37          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 4        | 0.36          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 4        | 0.36          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 4        | 0.36          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 15       | 0.36          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 15       | 0.36          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 15       | 0.36          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 16       | 0.36          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 16       | 0.36          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 16       | 0.36          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 3        | 0.36          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG12 | 3        | 0.36          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG13 | 3        | 0.36          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 19       | 0.36          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG12 | 19       | 0.36          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG13 | 19       | 0.36          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG11 | 19       | 0.36          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG12 | 19       | 0.36          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG13 | 19       | 0.36          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 4        | 0.36          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 4        | 0.36          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 4        | 0.36          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 4        | 0.36          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 4        | 0.36          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 4        | 0.36          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 4        | 0.36          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 4        | 0.36          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 4        | 0.36          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 4        | 0.36          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 4        | 0.36          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 4        | 0.36          |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD11  | 9        | 0.36          |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD12  | 9        | 0.36          |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD13  | 9        | 0.36          |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD11  | 9        | 0.36          |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD12  | 9        | 0.36          |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD13  | 9        | 0.36          |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD11  | 9        | 0.36          |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD12  | 9        | 0.36          |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD13  | 9        | 0.36          |
| (1,1737) | 1:15:A:SER:HB2   | 1:79:A:LEU:HD11  | 18       | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1737) | 1:15:A:SER:HB2   | 1:79:A:LEU:HD12  | 18       | 0.36          |
| (1,1737) | 1:15:A:SER:HB2   | 1:79:A:LEU:HD13  | 18       | 0.36          |
| (1,1737) | 1:15:A:SER:HB3   | 1:79:A:LEU:HD11  | 18       | 0.36          |
| (1,1737) | 1:15:A:SER:HB3   | 1:79:A:LEU:HD12  | 18       | 0.36          |
| (1,1737) | 1:15:A:SER:HB3   | 1:79:A:LEU:HD13  | 18       | 0.36          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 5        | 0.36          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 5        | 0.36          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 5        | 0.36          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 16       | 0.36          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 16       | 0.36          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 16       | 0.36          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD11  | 18       | 0.36          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD12  | 18       | 0.36          |
| (1,916)  | 1:37:A:LEU:HA    | 1:37:A:LEU:HD13  | 18       | 0.36          |
| (1,405)  | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB   | 16       | 0.36          |
| (1,405)  | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB   | 16       | 0.36          |
| (1,405)  | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB   | 16       | 0.36          |
| (1,405)  | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB   | 18       | 0.36          |
| (1,405)  | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB   | 18       | 0.36          |
| (1,405)  | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB   | 18       | 0.36          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG21   | 6        | 0.36          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG22   | 6        | 0.36          |
| (1,274)  | 1:5:A:MET:H      | 1:4:A:VAL:HG23   | 6        | 0.36          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 1        | 0.35          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 1        | 0.35          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 1        | 0.35          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 18       | 0.35          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG12 | 18       | 0.35          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG13 | 18       | 0.35          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 18       | 0.35          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 18       | 0.35          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 18       | 0.35          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 6        | 0.35          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 6        | 0.35          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 6        | 0.35          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 18       | 0.35          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 18       | 0.35          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 18       | 0.35          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 8        | 0.35          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 8        | 0.35          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 8        | 0.35          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 18       | 0.35          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2241) | 1:111:A:VAL:H   | 1:111:A:VAL:HG12 | 18       | 0.35          |
| (1,2241) | 1:111:A:VAL:H   | 1:111:A:VAL:HG13 | 18       | 0.35          |
| (1,1755) | 1:91:A:VAL:HG21 | 1:83:A:GLY:HA2   | 8        | 0.35          |
| (1,1755) | 1:91:A:VAL:HG21 | 1:83:A:GLY:HA3   | 8        | 0.35          |
| (1,1755) | 1:91:A:VAL:HG22 | 1:83:A:GLY:HA2   | 8        | 0.35          |
| (1,1755) | 1:91:A:VAL:HG22 | 1:83:A:GLY:HA3   | 8        | 0.35          |
| (1,1755) | 1:91:A:VAL:HG23 | 1:83:A:GLY:HA2   | 8        | 0.35          |
| (1,1755) | 1:91:A:VAL:HG23 | 1:83:A:GLY:HA3   | 8        | 0.35          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG21  | 16       | 0.35          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG22  | 16       | 0.35          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG23  | 16       | 0.35          |
| (1,921)  | 1:85:A:ASN:HB2  | 1:37:A:LEU:HD21  | 5        | 0.35          |
| (1,921)  | 1:85:A:ASN:HB2  | 1:37:A:LEU:HD22  | 5        | 0.35          |
| (1,921)  | 1:85:A:ASN:HB2  | 1:37:A:LEU:HD23  | 5        | 0.35          |
| (1,921)  | 1:85:A:ASN:HB3  | 1:37:A:LEU:HD21  | 5        | 0.35          |
| (1,921)  | 1:85:A:ASN:HB3  | 1:37:A:LEU:HD22  | 5        | 0.35          |
| (1,921)  | 1:85:A:ASN:HB3  | 1:37:A:LEU:HD23  | 5        | 0.35          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD11  | 1        | 0.35          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD12  | 1        | 0.35          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD13  | 1        | 0.35          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD11  | 10       | 0.35          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD12  | 10       | 0.35          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD13  | 10       | 0.35          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD11  | 11       | 0.35          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD12  | 11       | 0.35          |
| (1,916)  | 1:37:A:LEU:HA   | 1:37:A:LEU:HD13  | 11       | 0.35          |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG21  | 11       | 0.35          |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG22  | 11       | 0.35          |
| (1,812)  | 1:4:A:VAL:HG21  | 1:32:A:VAL:HG23  | 11       | 0.35          |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG21  | 11       | 0.35          |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG22  | 11       | 0.35          |
| (1,812)  | 1:4:A:VAL:HG22  | 1:32:A:VAL:HG23  | 11       | 0.35          |
| (1,812)  | 1:4:A:VAL:HG23  | 1:32:A:VAL:HG21  | 11       | 0.35          |
| (1,812)  | 1:4:A:VAL:HG23  | 1:32:A:VAL:HG22  | 11       | 0.35          |
| (1,812)  | 1:4:A:VAL:HG23  | 1:32:A:VAL:HG23  | 11       | 0.35          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG11  | 3        | 0.35          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG12  | 3        | 0.35          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG13  | 3        | 0.35          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG11  | 7        | 0.35          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG12  | 7        | 0.35          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG13  | 7        | 0.35          |
| (1,805)  | 1:6:A:PHE:HD1   | 1:32:A:VAL:HG11  | 10       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12  | 10       | 0.35          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13  | 10       | 0.35          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11  | 10       | 0.35          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12  | 10       | 0.35          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13  | 10       | 0.35          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA    | 18       | 0.35          |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA    | 18       | 0.35          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA    | 18       | 0.35          |
| (1,405)  | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB   | 14       | 0.35          |
| (1,405)  | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB   | 14       | 0.35          |
| (1,405)  | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB   | 14       | 0.35          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG11   | 5        | 0.35          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG12   | 5        | 0.35          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG13   | 5        | 0.35          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 10       | 0.35          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 10       | 0.35          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 10       | 0.35          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 10       | 0.35          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 10       | 0.35          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 10       | 0.35          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2   | 19       | 0.35          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3   | 19       | 0.35          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2   | 19       | 0.35          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3   | 19       | 0.35          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2   | 19       | 0.35          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3   | 19       | 0.35          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG11 | 14       | 0.34          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG12 | 14       | 0.34          |
| (1,2566) | 1:119:A:VAL:HA   | 1:123:A:VAL:HG13 | 14       | 0.34          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 4        | 0.34          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 4        | 0.34          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 4        | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 5        | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 5        | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 5        | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 6        | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 6        | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 6        | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 11       | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 11       | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 11       | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 12       | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 12       | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 12       | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 16       | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 16       | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 16       | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 20       | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 20       | 0.34          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 20       | 0.34          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD21  | 16       | 0.34          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD22  | 16       | 0.34          |
| (1,1814) | 1:91:A:VAL:H     | 1:86:A:LEU:HD23  | 16       | 0.34          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG21  | 17       | 0.34          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG22  | 17       | 0.34          |
| (1,1654) | 1:97:A:GLU:H     | 1:76:A:VAL:HG23  | 17       | 0.34          |
| (1,87)   | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD1  | 13       | 0.34          |
| (1,87)   | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD2  | 13       | 0.34          |
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD1  | 13       | 0.34          |
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD2  | 13       | 0.34          |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD1  | 13       | 0.34          |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD2  | 13       | 0.34          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 7        | 0.33          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 7        | 0.33          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 7        | 0.33          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 9        | 0.33          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 9        | 0.33          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 9        | 0.33          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 9        | 0.33          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 9        | 0.33          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 9        | 0.33          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 9        | 0.33          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 9        | 0.33          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 9        | 0.33          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 4        | 0.33          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 4        | 0.33          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 4        | 0.33          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 9        | 0.33          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 9        | 0.33          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 9        | 0.33          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 13       | 0.33          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 13       | 0.33          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 13       | 0.33          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 14       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 14       | 0.33          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 14       | 0.33          |
| (1,1756) | 1:86:A:LEU:HD11  | 1:84:A:VAL:HA    | 15       | 0.33          |
| (1,1756) | 1:86:A:LEU:HD12  | 1:84:A:VAL:HA    | 15       | 0.33          |
| (1,1756) | 1:86:A:LEU:HD13  | 1:84:A:VAL:HA    | 15       | 0.33          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG21  | 10       | 0.33          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG22  | 10       | 0.33          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG23  | 10       | 0.33          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 9        | 0.33          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 9        | 0.33          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 9        | 0.33          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 9        | 0.33          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 9        | 0.33          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 9        | 0.33          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11  | 15       | 0.33          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG12  | 15       | 0.33          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG13  | 15       | 0.33          |
| (1,532)  | 1:32:A:VAL:HG21  | 1:20:A:GLY:HA2   | 5        | 0.33          |
| (1,532)  | 1:32:A:VAL:HG21  | 1:20:A:GLY:HA3   | 5        | 0.33          |
| (1,532)  | 1:32:A:VAL:HG22  | 1:20:A:GLY:HA2   | 5        | 0.33          |
| (1,532)  | 1:32:A:VAL:HG22  | 1:20:A:GLY:HA3   | 5        | 0.33          |
| (1,532)  | 1:32:A:VAL:HG23  | 1:20:A:GLY:HA2   | 5        | 0.33          |
| (1,532)  | 1:32:A:VAL:HG23  | 1:20:A:GLY:HA3   | 5        | 0.33          |
| (1,87)   | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD1  | 3        | 0.33          |
| (1,87)   | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD2  | 3        | 0.33          |
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD1  | 3        | 0.33          |
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD2  | 3        | 0.33          |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD1  | 3        | 0.33          |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD2  | 3        | 0.33          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 9        | 0.32          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 9        | 0.32          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 9        | 0.32          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 16       | 0.32          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 16       | 0.32          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 16       | 0.32          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 6        | 0.32          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 6        | 0.32          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 6        | 0.32          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 6        | 0.32          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 6        | 0.32          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 6        | 0.32          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 6        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 6        | 0.32          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 6        | 0.32          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 19       | 0.32          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 19       | 0.32          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 19       | 0.32          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 19       | 0.32          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 19       | 0.32          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 19       | 0.32          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 19       | 0.32          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 19       | 0.32          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 19       | 0.32          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG21 | 18       | 0.32          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG22 | 18       | 0.32          |
| (1,2251) | 1:104:A:PRO:HA   | 1:111:A:VAL:HG23 | 18       | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 2        | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 2        | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 2        | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 3        | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 3        | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 3        | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 7        | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 7        | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 7        | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 10       | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 10       | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 10       | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 15       | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 15       | 0.32          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 15       | 0.32          |
| (1,2107) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HA   | 18       | 0.32          |
| (1,2107) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HA   | 18       | 0.32          |
| (1,2107) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HA   | 18       | 0.32          |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD11  | 16       | 0.32          |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD12  | 16       | 0.32          |
| (1,1796) | 1:91:A:VAL:HG21  | 1:86:A:LEU:HD13  | 16       | 0.32          |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD11  | 16       | 0.32          |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD12  | 16       | 0.32          |
| (1,1796) | 1:91:A:VAL:HG22  | 1:86:A:LEU:HD13  | 16       | 0.32          |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD11  | 16       | 0.32          |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD12  | 16       | 0.32          |
| (1,1796) | 1:91:A:VAL:HG23  | 1:86:A:LEU:HD13  | 16       | 0.32          |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA    | 3        | 0.32          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1776) | 1:37:A:LEU:HD12 | 1:86:A:LEU:HA    | 3        | 0.32          |
| (1,1776) | 1:37:A:LEU:HD13 | 1:86:A:LEU:HA    | 3        | 0.32          |
| (1,1456) | 1:7:A:VAL:HG21  | 1:65:A:ILE:HB    | 6        | 0.32          |
| (1,1456) | 1:7:A:VAL:HG22  | 1:65:A:ILE:HB    | 6        | 0.32          |
| (1,1456) | 1:7:A:VAL:HG23  | 1:65:A:ILE:HB    | 6        | 0.32          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD11  | 3        | 0.32          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD12  | 3        | 0.32          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD13  | 3        | 0.32          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG21 | 7        | 0.32          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG22 | 7        | 0.32          |
| (1,814)  | 1:25:A:LEU:HB2  | 1:123:A:VAL:HG23 | 7        | 0.32          |
| (1,814)  | 1:25:A:LEU:HB3  | 1:123:A:VAL:HG21 | 7        | 0.32          |
| (1,814)  | 1:25:A:LEU:HB3  | 1:123:A:VAL:HG22 | 7        | 0.32          |
| (1,814)  | 1:25:A:LEU:HB3  | 1:123:A:VAL:HG23 | 7        | 0.32          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG11  | 8        | 0.32          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG12  | 8        | 0.32          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG13  | 8        | 0.32          |
| (1,42)   | 1:86:A:LEU:HD11 | 1:90:A:TRP:HA    | 7        | 0.32          |
| (1,42)   | 1:86:A:LEU:HD12 | 1:90:A:TRP:HA    | 7        | 0.32          |
| (1,42)   | 1:86:A:LEU:HD13 | 1:90:A:TRP:HA    | 7        | 0.32          |
| (1,42)   | 1:86:A:LEU:HD11 | 1:90:A:TRP:HA    | 9        | 0.32          |
| (1,42)   | 1:86:A:LEU:HD12 | 1:90:A:TRP:HA    | 9        | 0.32          |
| (1,42)   | 1:86:A:LEU:HD13 | 1:90:A:TRP:HA    | 9        | 0.32          |
| (1,42)   | 1:86:A:LEU:HD11 | 1:90:A:TRP:HA    | 11       | 0.32          |
| (1,42)   | 1:86:A:LEU:HD12 | 1:90:A:TRP:HA    | 11       | 0.32          |
| (1,42)   | 1:86:A:LEU:HD13 | 1:90:A:TRP:HA    | 11       | 0.32          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG11 | 2        | 0.31          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG12 | 2        | 0.31          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG13 | 2        | 0.31          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG11 | 6        | 0.31          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG12 | 6        | 0.31          |
| (1,2562) | 1:99:A:TRP:HH2  | 1:123:A:VAL:HG13 | 6        | 0.31          |
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG21 | 13       | 0.31          |
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG22 | 13       | 0.31          |
| (1,2247) | 1:102:A:GLU:HB2 | 1:111:A:VAL:HG23 | 13       | 0.31          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG21 | 13       | 0.31          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG22 | 13       | 0.31          |
| (1,2247) | 1:102:A:GLU:HB3 | 1:111:A:VAL:HG23 | 13       | 0.31          |
| (1,2241) | 1:111:A:VAL:H   | 1:111:A:VAL:HG11 | 1        | 0.31          |
| (1,2241) | 1:111:A:VAL:H   | 1:111:A:VAL:HG12 | 1        | 0.31          |
| (1,2241) | 1:111:A:VAL:H   | 1:111:A:VAL:HG13 | 1        | 0.31          |
| (1,2241) | 1:111:A:VAL:H   | 1:111:A:VAL:HG11 | 17       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 17       | 0.31          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 17       | 0.31          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG11 | 19       | 0.31          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG12 | 19       | 0.31          |
| (1,2241) | 1:111:A:VAL:H    | 1:111:A:VAL:HG13 | 19       | 0.31          |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA    | 1        | 0.31          |
| (1,1776) | 1:37:A:LEU:HD12  | 1:86:A:LEU:HA    | 1        | 0.31          |
| (1,1776) | 1:37:A:LEU:HD13  | 1:86:A:LEU:HA    | 1        | 0.31          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD11  | 1        | 0.31          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12  | 1        | 0.31          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13  | 1        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11  | 4        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12  | 4        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13  | 4        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11  | 4        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12  | 4        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13  | 4        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG11  | 9        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG12  | 9        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD1    | 1:32:A:VAL:HG13  | 9        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG11  | 9        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG12  | 9        | 0.31          |
| (1,805)  | 1:6:A:PHE:HD2    | 1:32:A:VAL:HG13  | 9        | 0.31          |
| (1,405)  | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB   | 19       | 0.31          |
| (1,405)  | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB   | 19       | 0.31          |
| (1,405)  | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB   | 19       | 0.31          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG11   | 1        | 0.31          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG12   | 1        | 0.31          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG13   | 1        | 0.31          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG11   | 18       | 0.31          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG12   | 18       | 0.31          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG13   | 18       | 0.31          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ     | 11       | 0.31          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ     | 11       | 0.31          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ     | 11       | 0.31          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 4        | 0.31          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 4        | 0.31          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 4        | 0.31          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 4        | 0.31          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 4        | 0.31          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 4        | 0.31          |
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD1    | 9        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,91)   | 1:32:A:VAL:HG11  | 1:6:A:PHE:HD2    | 9        | 0.31          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD1    | 9        | 0.31          |
| (1,91)   | 1:32:A:VAL:HG12  | 1:6:A:PHE:HD2    | 9        | 0.31          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD1    | 9        | 0.31          |
| (1,91)   | 1:32:A:VAL:HG13  | 1:6:A:PHE:HD2    | 9        | 0.31          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H     | 6        | 0.3           |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H     | 6        | 0.3           |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H     | 6        | 0.3           |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 3        | 0.3           |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 3        | 0.3           |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 3        | 0.3           |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 6        | 0.3           |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 6        | 0.3           |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 6        | 0.3           |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 2        | 0.3           |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 2        | 0.3           |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 2        | 0.3           |
| (1,991)  | 1:57:A:ILE:H     | 1:42:A:VAL:HB    | 8        | 0.3           |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11  | 14       | 0.3           |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG12  | 14       | 0.3           |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG13  | 14       | 0.3           |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG2   | 9        | 0.3           |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG3   | 9        | 0.3           |
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG2   | 9        | 0.3           |
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG3   | 9        | 0.3           |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG2   | 9        | 0.3           |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG3   | 9        | 0.3           |
| (1,405)  | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB   | 6        | 0.3           |
| (1,405)  | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB   | 6        | 0.3           |
| (1,405)  | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB   | 6        | 0.3           |
| (1,405)  | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB   | 11       | 0.3           |
| (1,405)  | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB   | 11       | 0.3           |
| (1,405)  | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB   | 11       | 0.3           |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG21   | 20       | 0.3           |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG22   | 20       | 0.3           |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG23   | 20       | 0.3           |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 4        | 0.3           |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 4        | 0.3           |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 4        | 0.3           |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11   | 4        | 0.3           |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12   | 4        | 0.3           |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13   | 4        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11   | 4        | 0.3           |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12   | 4        | 0.3           |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13   | 4        | 0.3           |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 15       | 0.3           |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 15       | 0.3           |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 15       | 0.3           |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11   | 15       | 0.3           |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12   | 15       | 0.3           |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13   | 15       | 0.3           |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11   | 15       | 0.3           |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12   | 15       | 0.3           |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13   | 15       | 0.3           |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 10       | 0.29          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 10       | 0.29          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 10       | 0.29          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 13       | 0.29          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 13       | 0.29          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 13       | 0.29          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H     | 2        | 0.29          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H     | 2        | 0.29          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H     | 2        | 0.29          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H     | 18       | 0.29          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H     | 18       | 0.29          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H     | 18       | 0.29          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 2        | 0.29          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 2        | 0.29          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 2        | 0.29          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 17       | 0.29          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 17       | 0.29          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 17       | 0.29          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 9        | 0.29          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 9        | 0.29          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 9        | 0.29          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA   | 6        | 0.29          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA   | 6        | 0.29          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA   | 6        | 0.29          |
| (1,1803) | 1:96:A:PHE:HD1   | 1:86:A:LEU:HD11  | 17       | 0.29          |
| (1,1803) | 1:96:A:PHE:HD1   | 1:86:A:LEU:HD12  | 17       | 0.29          |
| (1,1803) | 1:96:A:PHE:HD1   | 1:86:A:LEU:HD13  | 17       | 0.29          |
| (1,1803) | 1:96:A:PHE:HD2   | 1:86:A:LEU:HD11  | 17       | 0.29          |
| (1,1803) | 1:96:A:PHE:HD2   | 1:86:A:LEU:HD12  | 17       | 0.29          |
| (1,1803) | 1:96:A:PHE:HD2   | 1:86:A:LEU:HD13  | 17       | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1796) | 1:91:A:VAL:HG21 | 1:86:A:LEU:HD11 | 11       | 0.29          |
| (1,1796) | 1:91:A:VAL:HG21 | 1:86:A:LEU:HD12 | 11       | 0.29          |
| (1,1796) | 1:91:A:VAL:HG21 | 1:86:A:LEU:HD13 | 11       | 0.29          |
| (1,1796) | 1:91:A:VAL:HG22 | 1:86:A:LEU:HD11 | 11       | 0.29          |
| (1,1796) | 1:91:A:VAL:HG22 | 1:86:A:LEU:HD12 | 11       | 0.29          |
| (1,1796) | 1:91:A:VAL:HG22 | 1:86:A:LEU:HD13 | 11       | 0.29          |
| (1,1796) | 1:91:A:VAL:HG23 | 1:86:A:LEU:HD11 | 11       | 0.29          |
| (1,1796) | 1:91:A:VAL:HG23 | 1:86:A:LEU:HD12 | 11       | 0.29          |
| (1,1796) | 1:91:A:VAL:HG23 | 1:86:A:LEU:HD13 | 11       | 0.29          |
| (1,1776) | 1:37:A:LEU:HD11 | 1:86:A:LEU:HA   | 9        | 0.29          |
| (1,1776) | 1:37:A:LEU:HD12 | 1:86:A:LEU:HA   | 9        | 0.29          |
| (1,1776) | 1:37:A:LEU:HD13 | 1:86:A:LEU:HA   | 9        | 0.29          |
| (1,1756) | 1:86:A:LEU:HD11 | 1:84:A:VAL:HA   | 17       | 0.29          |
| (1,1756) | 1:86:A:LEU:HD12 | 1:84:A:VAL:HA   | 17       | 0.29          |
| (1,1756) | 1:86:A:LEU:HD13 | 1:84:A:VAL:HA   | 17       | 0.29          |
| (1,1737) | 1:15:A:SER:HB2  | 1:79:A:LEU:HD11 | 8        | 0.29          |
| (1,1737) | 1:15:A:SER:HB2  | 1:79:A:LEU:HD12 | 8        | 0.29          |
| (1,1737) | 1:15:A:SER:HB2  | 1:79:A:LEU:HD13 | 8        | 0.29          |
| (1,1737) | 1:15:A:SER:HB3  | 1:79:A:LEU:HD11 | 8        | 0.29          |
| (1,1737) | 1:15:A:SER:HB3  | 1:79:A:LEU:HD12 | 8        | 0.29          |
| (1,1737) | 1:15:A:SER:HB3  | 1:79:A:LEU:HD13 | 8        | 0.29          |
| (1,1737) | 1:15:A:SER:HB2  | 1:79:A:LEU:HD11 | 15       | 0.29          |
| (1,1737) | 1:15:A:SER:HB2  | 1:79:A:LEU:HD12 | 15       | 0.29          |
| (1,1737) | 1:15:A:SER:HB2  | 1:79:A:LEU:HD13 | 15       | 0.29          |
| (1,1737) | 1:15:A:SER:HB3  | 1:79:A:LEU:HD11 | 15       | 0.29          |
| (1,1737) | 1:15:A:SER:HB3  | 1:79:A:LEU:HD12 | 15       | 0.29          |
| (1,1737) | 1:15:A:SER:HB3  | 1:79:A:LEU:HD13 | 15       | 0.29          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG21 | 3        | 0.29          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG22 | 3        | 0.29          |
| (1,1654) | 1:97:A:GLU:H    | 1:76:A:VAL:HG23 | 3        | 0.29          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD11 | 9        | 0.29          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD12 | 9        | 0.29          |
| (1,917)  | 1:86:A:LEU:HA   | 1:37:A:LEU:HD13 | 9        | 0.29          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG21 | 1        | 0.29          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG22 | 1        | 0.29          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG23 | 1        | 0.29          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG21 | 4        | 0.29          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG22 | 4        | 0.29          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG23 | 4        | 0.29          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG11 | 9        | 0.29          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG12 | 9        | 0.29          |
| (1,810)  | 1:33:A:THR:H    | 1:32:A:VAL:HG13 | 9        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11  | 10       | 0.29          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG12  | 10       | 0.29          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG13  | 10       | 0.29          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 14       | 0.29          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 14       | 0.29          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 14       | 0.29          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11   | 14       | 0.29          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12   | 14       | 0.29          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13   | 14       | 0.29          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11   | 14       | 0.29          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12   | 14       | 0.29          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13   | 14       | 0.29          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA    | 3        | 0.29          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA    | 3        | 0.29          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA    | 3        | 0.29          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H    | 13       | 0.28          |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H    | 13       | 0.28          |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H    | 13       | 0.28          |
| (1,2746) | 1:119:A:VAL:HG21 | 1:15:A:SER:HA    | 9        | 0.28          |
| (1,2746) | 1:119:A:VAL:HG22 | 1:15:A:SER:HA    | 9        | 0.28          |
| (1,2746) | 1:119:A:VAL:HG23 | 1:15:A:SER:HA    | 9        | 0.28          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 3        | 0.28          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 3        | 0.28          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 3        | 0.28          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 14       | 0.28          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 14       | 0.28          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 14       | 0.28          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG11 | 4        | 0.28          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG12 | 4        | 0.28          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG13 | 4        | 0.28          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 1        | 0.28          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 1        | 0.28          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 1        | 0.28          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 4        | 0.28          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 4        | 0.28          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 4        | 0.28          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 20       | 0.28          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 20       | 0.28          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 20       | 0.28          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 13       | 0.28          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 13       | 0.28          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 13       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 13       | 0.28          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 13       | 0.28          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 13       | 0.28          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 13       | 0.28          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 13       | 0.28          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 13       | 0.28          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 18       | 0.28          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 18       | 0.28          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 18       | 0.28          |
| (1,1737) | 1:15:A:SER:HB2   | 1:79:A:LEU:HD11  | 10       | 0.28          |
| (1,1737) | 1:15:A:SER:HB2   | 1:79:A:LEU:HD12  | 10       | 0.28          |
| (1,1737) | 1:15:A:SER:HB2   | 1:79:A:LEU:HD13  | 10       | 0.28          |
| (1,1737) | 1:15:A:SER:HB3   | 1:79:A:LEU:HD11  | 10       | 0.28          |
| (1,1737) | 1:15:A:SER:HB3   | 1:79:A:LEU:HD12  | 10       | 0.28          |
| (1,1737) | 1:15:A:SER:HB3   | 1:79:A:LEU:HD13  | 10       | 0.28          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG21  | 12       | 0.28          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG22  | 12       | 0.28          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG23  | 12       | 0.28          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11  | 12       | 0.28          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG12  | 12       | 0.28          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG13  | 12       | 0.28          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB1   | 13       | 0.28          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB2   | 13       | 0.28          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB3   | 13       | 0.28          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB1   | 13       | 0.28          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB2   | 13       | 0.28          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB3   | 13       | 0.28          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB1   | 13       | 0.28          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB2   | 13       | 0.28          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB3   | 13       | 0.28          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA    | 3        | 0.28          |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA    | 3        | 0.28          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA    | 3        | 0.28          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA    | 14       | 0.28          |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA    | 14       | 0.28          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA    | 14       | 0.28          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG21   | 11       | 0.28          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG22   | 11       | 0.28          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG23   | 11       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 2        | 0.28          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 2        | 0.28          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 2        | 0.28          |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11 | 2        | 0.28          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12 | 2        | 0.28          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13 | 2        | 0.28          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11 | 2        | 0.28          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12 | 2        | 0.28          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13 | 2        | 0.28          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11 | 11       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12 | 11       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13 | 11       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11 | 11       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12 | 11       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13 | 11       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11 | 11       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12 | 11       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13 | 11       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11 | 16       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12 | 16       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13 | 16       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11 | 16       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12 | 16       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13 | 16       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11 | 16       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12 | 16       | 0.28          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13 | 16       | 0.28          |
| (1,145)  | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ   | 20       | 0.28          |
| (1,145)  | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ   | 20       | 0.28          |
| (1,145)  | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ   | 20       | 0.28          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA  | 2        | 0.28          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA  | 2        | 0.28          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA  | 2        | 0.28          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H  | 11       | 0.27          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H  | 11       | 0.27          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H  | 11       | 0.27          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H  | 15       | 0.27          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H  | 15       | 0.27          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H  | 15       | 0.27          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H  | 6        | 0.27          |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H  | 6        | 0.27          |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H  | 6        | 0.27          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H  | 9        | 0.27          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H  | 9        | 0.27          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H   | 3        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H     | 3        | 0.27          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H     | 3        | 0.27          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H     | 4        | 0.27          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H     | 4        | 0.27          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H     | 4        | 0.27          |
| (1,2653) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HB   | 13       | 0.27          |
| (1,2653) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HB   | 13       | 0.27          |
| (1,2653) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HB   | 13       | 0.27          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 12       | 0.27          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 12       | 0.27          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 12       | 0.27          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 14       | 0.27          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 14       | 0.27          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 14       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 5        | 0.27          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 5        | 0.27          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 5        | 0.27          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 5        | 0.27          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 5        | 0.27          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 5        | 0.27          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 5        | 0.27          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 5        | 0.27          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 5        | 0.27          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 11       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 11       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 11       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 11       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 11       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 11       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 11       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 11       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 11       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 16       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 16       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 16       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 16       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 16       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 16       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 16       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 16       | 0.27          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 16       | 0.27          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 8        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 8        | 0.27          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 8        | 0.27          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 11       | 0.27          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 11       | 0.27          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 11       | 0.27          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA   | 13       | 0.27          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA   | 13       | 0.27          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA   | 13       | 0.27          |
| (1,1756) | 1:86:A:LEU:HD11  | 1:84:A:VAL:HA    | 9        | 0.27          |
| (1,1756) | 1:86:A:LEU:HD12  | 1:84:A:VAL:HA    | 9        | 0.27          |
| (1,1756) | 1:86:A:LEU:HD13  | 1:84:A:VAL:HA    | 9        | 0.27          |
| (1,405)  | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB   | 9        | 0.27          |
| (1,405)  | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB   | 9        | 0.27          |
| (1,405)  | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB   | 9        | 0.27          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG21   | 14       | 0.27          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG22   | 14       | 0.27          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG23   | 14       | 0.27          |
| (1,262)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG21   | 11       | 0.27          |
| (1,262)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG22   | 11       | 0.27          |
| (1,262)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG23   | 11       | 0.27          |
| (1,262)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG21   | 11       | 0.27          |
| (1,262)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG22   | 11       | 0.27          |
| (1,262)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG23   | 11       | 0.27          |
| (1,262)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG21   | 11       | 0.27          |
| (1,262)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG22   | 11       | 0.27          |
| (1,262)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG23   | 11       | 0.27          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA    | 8        | 0.27          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA    | 8        | 0.27          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA    | 8        | 0.27          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA    | 19       | 0.27          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA    | 19       | 0.27          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA    | 19       | 0.27          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 9        | 0.26          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 9        | 0.26          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 9        | 0.26          |
| (1,2649) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HA   | 13       | 0.26          |
| (1,2649) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HA   | 13       | 0.26          |
| (1,2649) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HA   | 13       | 0.26          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 5        | 0.26          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 5        | 0.26          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 5        | 0.26          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 8        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 8        | 0.26          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 8        | 0.26          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 19       | 0.26          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 19       | 0.26          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 19       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 10       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 10       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 10       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 10       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 10       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 10       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 18       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 18       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 18       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 18       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 18       | 0.26          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 18       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 10       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 10       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 10       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 10       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 10       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 10       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 10       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 10       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 10       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 20       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 20       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 20       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 20       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 20       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 20       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 20       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 20       | 0.26          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 20       | 0.26          |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG21 | 1        | 0.26          |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG22 | 1        | 0.26          |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG23 | 1        | 0.26          |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG21 | 1        | 0.26          |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG22 | 1        | 0.26          |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG23 | 1        | 0.26          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 5        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 5        | 0.26          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 5        | 0.26          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 6        | 0.26          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 6        | 0.26          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 6        | 0.26          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 7        | 0.26          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 7        | 0.26          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 7        | 0.26          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 20       | 0.26          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 20       | 0.26          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 20       | 0.26          |
| (1,2176) | 1:109:A:LEU:HD21 | 1:108:A:SER:HA   | 15       | 0.26          |
| (1,2176) | 1:109:A:LEU:HD22 | 1:108:A:SER:HA   | 15       | 0.26          |
| (1,2176) | 1:109:A:LEU:HD23 | 1:108:A:SER:HA   | 15       | 0.26          |
| (1,1734) | 1:119:A:VAL:HG21 | 1:79:A:LEU:HD11  | 1        | 0.26          |
| (1,1734) | 1:119:A:VAL:HG21 | 1:79:A:LEU:HD12  | 1        | 0.26          |
| (1,1734) | 1:119:A:VAL:HG21 | 1:79:A:LEU:HD13  | 1        | 0.26          |
| (1,1734) | 1:119:A:VAL:HG22 | 1:79:A:LEU:HD11  | 1        | 0.26          |
| (1,1734) | 1:119:A:VAL:HG22 | 1:79:A:LEU:HD12  | 1        | 0.26          |
| (1,1734) | 1:119:A:VAL:HG22 | 1:79:A:LEU:HD13  | 1        | 0.26          |
| (1,1734) | 1:119:A:VAL:HG23 | 1:79:A:LEU:HD11  | 1        | 0.26          |
| (1,1734) | 1:119:A:VAL:HG23 | 1:79:A:LEU:HD12  | 1        | 0.26          |
| (1,1734) | 1:119:A:VAL:HG23 | 1:79:A:LEU:HD13  | 1        | 0.26          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD21  | 8        | 0.26          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD22  | 8        | 0.26          |
| (1,921)  | 1:85:A:ASN:HB2   | 1:37:A:LEU:HD23  | 8        | 0.26          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD21  | 8        | 0.26          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD22  | 8        | 0.26          |
| (1,921)  | 1:85:A:ASN:HB3   | 1:37:A:LEU:HD23  | 8        | 0.26          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD11  | 6        | 0.26          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD12  | 6        | 0.26          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD13  | 6        | 0.26          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD11  | 6        | 0.26          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD12  | 6        | 0.26          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD13  | 6        | 0.26          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD11  | 6        | 0.26          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD12  | 6        | 0.26          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD13  | 6        | 0.26          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG21  | 16       | 0.26          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG22  | 16       | 0.26          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG23  | 16       | 0.26          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11  | 6        | 0.26          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,810) | 1:33:A:THR:H     | 1:32:A:VAL:HG12 | 6        | 0.26          |
| (1,810) | 1:33:A:THR:H     | 1:32:A:VAL:HG13 | 6        | 0.26          |
| (1,797) | 1:30:A:ILE:HD11  | 1:32:A:VAL:HG11 | 5        | 0.26          |
| (1,797) | 1:30:A:ILE:HD11  | 1:32:A:VAL:HG12 | 5        | 0.26          |
| (1,797) | 1:30:A:ILE:HD11  | 1:32:A:VAL:HG13 | 5        | 0.26          |
| (1,797) | 1:30:A:ILE:HD12  | 1:32:A:VAL:HG11 | 5        | 0.26          |
| (1,797) | 1:30:A:ILE:HD12  | 1:32:A:VAL:HG12 | 5        | 0.26          |
| (1,797) | 1:30:A:ILE:HD12  | 1:32:A:VAL:HG13 | 5        | 0.26          |
| (1,797) | 1:30:A:ILE:HD13  | 1:32:A:VAL:HG11 | 5        | 0.26          |
| (1,797) | 1:30:A:ILE:HD13  | 1:32:A:VAL:HG12 | 5        | 0.26          |
| (1,797) | 1:30:A:ILE:HD13  | 1:32:A:VAL:HG13 | 5        | 0.26          |
| (1,405) | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB  | 2        | 0.26          |
| (1,405) | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB  | 2        | 0.26          |
| (1,405) | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB  | 2        | 0.26          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG21  | 3        | 0.26          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG22  | 3        | 0.26          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG23  | 3        | 0.26          |
| (1,264) | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG21  | 17       | 0.26          |
| (1,264) | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG22  | 17       | 0.26          |
| (1,264) | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG23  | 17       | 0.26          |
| (1,264) | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG21  | 17       | 0.26          |
| (1,264) | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG22  | 17       | 0.26          |
| (1,264) | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG23  | 17       | 0.26          |
| (1,264) | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG21  | 17       | 0.26          |
| (1,264) | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG22  | 17       | 0.26          |
| (1,264) | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG23  | 17       | 0.26          |
| (1,262) | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG21  | 14       | 0.26          |
| (1,262) | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG22  | 14       | 0.26          |
| (1,262) | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG23  | 14       | 0.26          |
| (1,262) | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG21  | 14       | 0.26          |
| (1,262) | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG22  | 14       | 0.26          |
| (1,262) | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG23  | 14       | 0.26          |
| (1,262) | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG21  | 14       | 0.26          |
| (1,262) | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG22  | 14       | 0.26          |
| (1,262) | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG23  | 14       | 0.26          |
| (1,262) | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG21  | 20       | 0.26          |
| (1,262) | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG22  | 20       | 0.26          |
| (1,262) | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG23  | 20       | 0.26          |
| (1,262) | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG21  | 20       | 0.26          |
| (1,262) | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG22  | 20       | 0.26          |
| (1,262) | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG23  | 20       | 0.26          |
| (1,262) | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG21  | 20       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,262)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG22   | 20       | 0.26          |
| (1,262)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG23   | 20       | 0.26          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 5        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 5        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 5        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11   | 5        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12   | 5        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13   | 5        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11   | 5        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12   | 5        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13   | 5        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 9        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 9        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 9        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11   | 9        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12   | 9        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13   | 9        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11   | 9        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12   | 9        | 0.26          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13   | 9        | 0.26          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 2        | 0.25          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 2        | 0.25          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 2        | 0.25          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H     | 5        | 0.25          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H     | 5        | 0.25          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H     | 5        | 0.25          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H     | 17       | 0.25          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H     | 17       | 0.25          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H     | 17       | 0.25          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H     | 19       | 0.25          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H     | 19       | 0.25          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H     | 19       | 0.25          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11  | 17       | 0.25          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12  | 17       | 0.25          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13  | 17       | 0.25          |
| (1,2746) | 1:119:A:VAL:HG21 | 1:15:A:SER:HA    | 7        | 0.25          |
| (1,2746) | 1:119:A:VAL:HG22 | 1:15:A:SER:HA    | 7        | 0.25          |
| (1,2746) | 1:119:A:VAL:HG23 | 1:15:A:SER:HA    | 7        | 0.25          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG11 | 3        | 0.25          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG12 | 3        | 0.25          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG13 | 3        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 3        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 3        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 3        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 3        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 3        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 3        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 6        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 6        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 6        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 6        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 6        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 6        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 9        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 9        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 9        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 9        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 9        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 9        | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 14       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 14       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 14       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 14       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 14       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 14       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 15       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 15       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 15       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 15       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 15       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 15       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 17       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 17       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 17       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 17       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 17       | 0.25          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 17       | 0.25          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 15       | 0.25          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 15       | 0.25          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 15       | 0.25          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 15       | 0.25          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 15       | 0.25          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 15       | 0.25          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 15       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 15       | 0.25          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 15       | 0.25          |
| (1,2246) | 1:114:A:THR:HG21 | 1:111:A:VAL:HG21 | 18       | 0.25          |
| (1,2246) | 1:114:A:THR:HG21 | 1:111:A:VAL:HG22 | 18       | 0.25          |
| (1,2246) | 1:114:A:THR:HG21 | 1:111:A:VAL:HG23 | 18       | 0.25          |
| (1,2246) | 1:114:A:THR:HG22 | 1:111:A:VAL:HG21 | 18       | 0.25          |
| (1,2246) | 1:114:A:THR:HG22 | 1:111:A:VAL:HG22 | 18       | 0.25          |
| (1,2246) | 1:114:A:THR:HG22 | 1:111:A:VAL:HG23 | 18       | 0.25          |
| (1,2246) | 1:114:A:THR:HG23 | 1:111:A:VAL:HG21 | 18       | 0.25          |
| (1,2246) | 1:114:A:THR:HG23 | 1:111:A:VAL:HG22 | 18       | 0.25          |
| (1,2246) | 1:114:A:THR:HG23 | 1:111:A:VAL:HG23 | 18       | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 2        | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 2        | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 2        | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 3        | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 3        | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 3        | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 17       | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 17       | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 17       | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 19       | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 19       | 0.25          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 19       | 0.25          |
| (1,928)  | 1:40:A:SER:HA    | 1:38:A:GLU:HA    | 16       | 0.25          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB1   | 10       | 0.25          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB2   | 10       | 0.25          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB3   | 10       | 0.25          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB1   | 10       | 0.25          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB2   | 10       | 0.25          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB3   | 10       | 0.25          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB1   | 10       | 0.25          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB2   | 10       | 0.25          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB3   | 10       | 0.25          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2   | 11       | 0.25          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3   | 11       | 0.25          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2   | 11       | 0.25          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3   | 11       | 0.25          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 19       | 0.25          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 19       | 0.25          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 19       | 0.25          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11   | 19       | 0.25          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12   | 19       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13   | 19       | 0.25          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11   | 19       | 0.25          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12   | 19       | 0.25          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13   | 19       | 0.25          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG11   | 4        | 0.25          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG12   | 4        | 0.25          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG13   | 4        | 0.25          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG11   | 8        | 0.25          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG12   | 8        | 0.25          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG13   | 8        | 0.25          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2   | 11       | 0.25          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3   | 11       | 0.25          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2   | 11       | 0.25          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3   | 11       | 0.25          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2   | 11       | 0.25          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3   | 11       | 0.25          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 10       | 0.24          |
| (1,3765) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 10       | 0.24          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 10       | 0.24          |
| (1,3765) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 10       | 0.24          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 10       | 0.24          |
| (1,3765) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 10       | 0.24          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE21 | 10       | 0.24          |
| (1,3720) | 1:111:A:VAL:HG21 | 1:107:A:GLN:HE22 | 10       | 0.24          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE21 | 10       | 0.24          |
| (1,3720) | 1:111:A:VAL:HG22 | 1:107:A:GLN:HE22 | 10       | 0.24          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE21 | 10       | 0.24          |
| (1,3720) | 1:111:A:VAL:HG23 | 1:107:A:GLN:HE22 | 10       | 0.24          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 20       | 0.24          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 20       | 0.24          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 20       | 0.24          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H     | 14       | 0.24          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H     | 14       | 0.24          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H     | 14       | 0.24          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 4        | 0.24          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 4        | 0.24          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 4        | 0.24          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 12       | 0.24          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 12       | 0.24          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 12       | 0.24          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 12       | 0.24          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 12       | 0.24          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2431) | 1:122:A:ARG:HD3 | 1:119:A:VAL:HG23 | 12       | 0.24          |
| (1,2426) | 1:21:A:PHE:HE1  | 1:119:A:VAL:HG21 | 18       | 0.24          |
| (1,2426) | 1:21:A:PHE:HE1  | 1:119:A:VAL:HG22 | 18       | 0.24          |
| (1,2426) | 1:21:A:PHE:HE1  | 1:119:A:VAL:HG23 | 18       | 0.24          |
| (1,2426) | 1:21:A:PHE:HE2  | 1:119:A:VAL:HG21 | 18       | 0.24          |
| (1,2426) | 1:21:A:PHE:HE2  | 1:119:A:VAL:HG22 | 18       | 0.24          |
| (1,2426) | 1:21:A:PHE:HE2  | 1:119:A:VAL:HG23 | 18       | 0.24          |
| (1,2416) | 1:6:A:PHE:HD1   | 1:126:A:LEU:HD11 | 1        | 0.24          |
| (1,2416) | 1:6:A:PHE:HD1   | 1:126:A:LEU:HD12 | 1        | 0.24          |
| (1,2416) | 1:6:A:PHE:HD1   | 1:126:A:LEU:HD13 | 1        | 0.24          |
| (1,2416) | 1:6:A:PHE:HD2   | 1:126:A:LEU:HD11 | 1        | 0.24          |
| (1,2416) | 1:6:A:PHE:HD2   | 1:126:A:LEU:HD12 | 1        | 0.24          |
| (1,2416) | 1:6:A:PHE:HD2   | 1:126:A:LEU:HD13 | 1        | 0.24          |
| (1,2416) | 1:6:A:PHE:HD1   | 1:126:A:LEU:HD11 | 2        | 0.24          |
| (1,2416) | 1:6:A:PHE:HD1   | 1:126:A:LEU:HD12 | 2        | 0.24          |
| (1,2416) | 1:6:A:PHE:HD1   | 1:126:A:LEU:HD13 | 2        | 0.24          |
| (1,2416) | 1:6:A:PHE:HD2   | 1:126:A:LEU:HD11 | 2        | 0.24          |
| (1,2416) | 1:6:A:PHE:HD2   | 1:126:A:LEU:HD12 | 2        | 0.24          |
| (1,2416) | 1:6:A:PHE:HD2   | 1:126:A:LEU:HD13 | 2        | 0.24          |
| (1,2245) | 1:104:A:PRO:HB2 | 1:111:A:VAL:HG21 | 8        | 0.24          |
| (1,2245) | 1:104:A:PRO:HB2 | 1:111:A:VAL:HG22 | 8        | 0.24          |
| (1,2245) | 1:104:A:PRO:HB2 | 1:111:A:VAL:HG23 | 8        | 0.24          |
| (1,2245) | 1:104:A:PRO:HB3 | 1:111:A:VAL:HG21 | 8        | 0.24          |
| (1,2245) | 1:104:A:PRO:HB3 | 1:111:A:VAL:HG22 | 8        | 0.24          |
| (1,2245) | 1:104:A:PRO:HB3 | 1:111:A:VAL:HG23 | 8        | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD21 | 1        | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD22 | 1        | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD23 | 1        | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD21 | 4        | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD22 | 4        | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD23 | 4        | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD21 | 12       | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD22 | 12       | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD23 | 12       | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD21 | 13       | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD22 | 13       | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD23 | 13       | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD21 | 16       | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD22 | 16       | 0.24          |
| (1,2207) | 1:109:A:LEU:HA  | 1:109:A:LEU:HD23 | 16       | 0.24          |
| (1,2124) | 1:4:A:VAL:HG21  | 1:126:A:LEU:HG   | 10       | 0.24          |
| (1,2124) | 1:4:A:VAL:HG22  | 1:126:A:LEU:HG   | 10       | 0.24          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2124) | 1:4:A:VAL:HG23   | 1:126:A:LEU:HG  | 10       | 0.24          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2  | 5        | 0.24          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3  | 5        | 0.24          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2  | 10       | 0.24          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3  | 10       | 0.24          |
| (1,1756) | 1:86:A:LEU:HD11  | 1:84:A:VAL:HA   | 14       | 0.24          |
| (1,1756) | 1:86:A:LEU:HD12  | 1:84:A:VAL:HA   | 14       | 0.24          |
| (1,1756) | 1:86:A:LEU:HD13  | 1:84:A:VAL:HA   | 14       | 0.24          |
| (1,1756) | 1:86:A:LEU:HD11  | 1:84:A:VAL:HA   | 18       | 0.24          |
| (1,1756) | 1:86:A:LEU:HD12  | 1:84:A:VAL:HA   | 18       | 0.24          |
| (1,1756) | 1:86:A:LEU:HD13  | 1:84:A:VAL:HA   | 18       | 0.24          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG11 | 8        | 0.24          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG12 | 8        | 0.24          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG13 | 8        | 0.24          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG11 | 8        | 0.24          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG12 | 8        | 0.24          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG13 | 8        | 0.24          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG11 | 8        | 0.24          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG12 | 8        | 0.24          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG13 | 8        | 0.24          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG11 | 8        | 0.24          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG12 | 8        | 0.24          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG13 | 8        | 0.24          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG11 | 8        | 0.24          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG12 | 8        | 0.24          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG13 | 8        | 0.24          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG11 | 8        | 0.24          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG12 | 8        | 0.24          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG13 | 8        | 0.24          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11 | 16       | 0.24          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG12 | 16       | 0.24          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG13 | 16       | 0.24          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA   | 4        | 0.24          |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA   | 4        | 0.24          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA   | 4        | 0.24          |
| (1,264)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG21  | 7        | 0.24          |
| (1,264)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG22  | 7        | 0.24          |
| (1,264)  | 1:75:A:VAL:HG21  | 1:4:A:VAL:HG23  | 7        | 0.24          |
| (1,264)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG21  | 7        | 0.24          |
| (1,264)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG22  | 7        | 0.24          |
| (1,264)  | 1:75:A:VAL:HG22  | 1:4:A:VAL:HG23  | 7        | 0.24          |
| (1,264)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG21  | 7        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,264)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG22   | 7        | 0.24          |
| (1,264)  | 1:75:A:VAL:HG23  | 1:4:A:VAL:HG23   | 7        | 0.24          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 8        | 0.24          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 8        | 0.24          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 8        | 0.24          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11   | 8        | 0.24          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12   | 8        | 0.24          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13   | 8        | 0.24          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11   | 8        | 0.24          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12   | 8        | 0.24          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13   | 8        | 0.24          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11   | 20       | 0.24          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12   | 20       | 0.24          |
| (1,261)  | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13   | 20       | 0.24          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11   | 20       | 0.24          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12   | 20       | 0.24          |
| (1,261)  | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13   | 20       | 0.24          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11   | 20       | 0.24          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12   | 20       | 0.24          |
| (1,261)  | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13   | 20       | 0.24          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA    | 4        | 0.24          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA    | 4        | 0.24          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA    | 4        | 0.24          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA    | 10       | 0.24          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA    | 10       | 0.24          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA    | 10       | 0.24          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA    | 18       | 0.24          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA    | 18       | 0.24          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA    | 18       | 0.24          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 17       | 0.23          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 17       | 0.23          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 17       | 0.23          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H    | 9        | 0.23          |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H    | 9        | 0.23          |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H    | 9        | 0.23          |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG11 | 20       | 0.23          |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG12 | 20       | 0.23          |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG13 | 20       | 0.23          |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG11 | 20       | 0.23          |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG12 | 20       | 0.23          |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG13 | 20       | 0.23          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG11 | 12       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG12 | 12       | 0.23          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG13 | 12       | 0.23          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG11 | 18       | 0.23          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG12 | 18       | 0.23          |
| (1,2558) | 1:123:A:VAL:H    | 1:123:A:VAL:HG13 | 18       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 2        | 0.23          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 2        | 0.23          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 2        | 0.23          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 2        | 0.23          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 2        | 0.23          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 2        | 0.23          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 11       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 11       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 11       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 11       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 11       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 11       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 13       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 13       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 13       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 13       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 13       | 0.23          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 13       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 3        | 0.23          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 3        | 0.23          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 3        | 0.23          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 3        | 0.23          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 3        | 0.23          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 3        | 0.23          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 19       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 19       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 19       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 19       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 19       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 19       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 20       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 20       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 20       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 20       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 20       | 0.23          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 20       | 0.23          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 20       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 20       | 0.23          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 1        | 0.23          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 1        | 0.23          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 1        | 0.23          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 1        | 0.23          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 1        | 0.23          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 1        | 0.23          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 1        | 0.23          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 1        | 0.23          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 1        | 0.23          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 14       | 0.23          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 14       | 0.23          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 14       | 0.23          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA   | 3        | 0.23          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA   | 3        | 0.23          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA   | 3        | 0.23          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA   | 14       | 0.23          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA   | 14       | 0.23          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA   | 14       | 0.23          |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA    | 18       | 0.23          |
| (1,1776) | 1:37:A:LEU:HD12  | 1:86:A:LEU:HA    | 18       | 0.23          |
| (1,1776) | 1:37:A:LEU:HD13  | 1:86:A:LEU:HA    | 18       | 0.23          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG11  | 10       | 0.23          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG12  | 10       | 0.23          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG13  | 10       | 0.23          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG11  | 10       | 0.23          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG12  | 10       | 0.23          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG13  | 10       | 0.23          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG11  | 10       | 0.23          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG12  | 10       | 0.23          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG13  | 10       | 0.23          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG11  | 1        | 0.23          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG12  | 1        | 0.23          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG13  | 1        | 0.23          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG11  | 1        | 0.23          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG12  | 1        | 0.23          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG13  | 1        | 0.23          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG11  | 1        | 0.23          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG12  | 1        | 0.23          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG13  | 1        | 0.23          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD11  | 18       | 0.23          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12  | 18       | 0.23          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,917) | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13 | 18       | 0.23          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG21 | 9        | 0.23          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG22 | 9        | 0.23          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG23 | 9        | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11  | 3        | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12  | 3        | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13  | 3        | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11  | 3        | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12  | 3        | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13  | 3        | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11  | 3        | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12  | 3        | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13  | 3        | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11  | 10       | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12  | 10       | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13  | 10       | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11  | 10       | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12  | 10       | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13  | 10       | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11  | 10       | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12  | 10       | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13  | 10       | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11  | 12       | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12  | 12       | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13  | 12       | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11  | 12       | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12  | 12       | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13  | 12       | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11  | 12       | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12  | 12       | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13  | 12       | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11  | 18       | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12  | 18       | 0.23          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13  | 18       | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11  | 18       | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12  | 18       | 0.23          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13  | 18       | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11  | 18       | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12  | 18       | 0.23          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13  | 18       | 0.23          |
| (1,87)  | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD1 | 12       | 0.23          |
| (1,87)  | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD2 | 12       | 0.23          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD1 | 12       | 0.23          |
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD2 | 12       | 0.23          |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD1 | 12       | 0.23          |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD2 | 12       | 0.23          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2  | 1        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3  | 1        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2  | 1        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3  | 1        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2  | 1        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3  | 1        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2  | 2        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3  | 2        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2  | 2        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3  | 2        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2  | 2        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3  | 2        | 0.23          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2  | 10       | 0.23          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3  | 10       | 0.23          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2  | 10       | 0.23          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3  | 10       | 0.23          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2  | 10       | 0.23          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3  | 10       | 0.23          |
| (1,42)   | 1:86:A:LEU:HD11  | 1:90:A:TRP:HA   | 1        | 0.23          |
| (1,42)   | 1:86:A:LEU:HD12  | 1:90:A:TRP:HA   | 1        | 0.23          |
| (1,42)   | 1:86:A:LEU:HD13  | 1:90:A:TRP:HA   | 1        | 0.23          |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD21 | 13       | 0.22          |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD22 | 13       | 0.22          |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD21 | 13       | 0.22          |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD22 | 13       | 0.22          |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD21 | 13       | 0.22          |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD22 | 13       | 0.22          |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD21 | 13       | 0.22          |
| (1,3740) | 1:37:A:LEU:HD21  | 1:85:A:ASN:HD22 | 13       | 0.22          |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD21 | 13       | 0.22          |
| (1,3740) | 1:37:A:LEU:HD22  | 1:85:A:ASN:HD22 | 13       | 0.22          |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD21 | 13       | 0.22          |
| (1,3740) | 1:37:A:LEU:HD23  | 1:85:A:ASN:HD22 | 13       | 0.22          |
| (1,3559) | 1:111:A:VAL:HG21 | 1:115:A:VAL:H   | 9        | 0.22          |
| (1,3559) | 1:111:A:VAL:HG22 | 1:115:A:VAL:H   | 9        | 0.22          |
| (1,3559) | 1:111:A:VAL:HG23 | 1:115:A:VAL:H   | 9        | 0.22          |
| (1,3472) | 1:79:A:LEU:HD21  | 1:99:A:TRP:H    | 8        | 0.22          |
| (1,3472) | 1:79:A:LEU:HD22  | 1:99:A:TRP:H    | 8        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3472) | 1:79:A:LEU:HD23  | 1:99:A:TRP:H     | 8        | 0.22          |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H     | 1        | 0.22          |
| (1,2754) | 1:79:A:LEU:HD11  | 1:15:A:SER:HB2   | 16       | 0.22          |
| (1,2754) | 1:79:A:LEU:HD11  | 1:15:A:SER:HB3   | 16       | 0.22          |
| (1,2754) | 1:79:A:LEU:HD12  | 1:15:A:SER:HB2   | 16       | 0.22          |
| (1,2754) | 1:79:A:LEU:HD12  | 1:15:A:SER:HB3   | 16       | 0.22          |
| (1,2754) | 1:79:A:LEU:HD13  | 1:15:A:SER:HB2   | 16       | 0.22          |
| (1,2754) | 1:79:A:LEU:HD13  | 1:15:A:SER:HB3   | 16       | 0.22          |
| (1,2754) | 1:79:A:LEU:HD11  | 1:15:A:SER:HB2   | 16       | 0.22          |
| (1,2754) | 1:79:A:LEU:HD11  | 1:15:A:SER:HB3   | 16       | 0.22          |
| (1,2754) | 1:79:A:LEU:HD12  | 1:15:A:SER:HB2   | 16       | 0.22          |
| (1,2754) | 1:79:A:LEU:HD12  | 1:15:A:SER:HB3   | 16       | 0.22          |
| (1,2754) | 1:79:A:LEU:HD13  | 1:15:A:SER:HB2   | 16       | 0.22          |
| (1,2754) | 1:79:A:LEU:HD13  | 1:15:A:SER:HB3   | 16       | 0.22          |
| (1,2649) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HA   | 7        | 0.22          |
| (1,2649) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HA   | 7        | 0.22          |
| (1,2649) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HA   | 7        | 0.22          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG11 | 5        | 0.22          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG12 | 5        | 0.22          |
| (1,2562) | 1:99:A:TRP:HH2   | 1:123:A:VAL:HG13 | 5        | 0.22          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 16       | 0.22          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 16       | 0.22          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 16       | 0.22          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 16       | 0.22          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 16       | 0.22          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 16       | 0.22          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 9        | 0.22          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 9        | 0.22          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 9        | 0.22          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 9        | 0.22          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 9        | 0.22          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 9        | 0.22          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 11       | 0.22          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 11       | 0.22          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 11       | 0.22          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 11       | 0.22          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 11       | 0.22          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 11       | 0.22          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 13       | 0.22          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 13       | 0.22          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 13       | 0.22          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 13       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 13       | 0.22          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 13       | 0.22          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 14       | 0.22          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 14       | 0.22          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 14       | 0.22          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 14       | 0.22          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 14       | 0.22          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 14       | 0.22          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 14       | 0.22          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 14       | 0.22          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 14       | 0.22          |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG21 | 9        | 0.22          |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG22 | 9        | 0.22          |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG23 | 9        | 0.22          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 10       | 0.22          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 10       | 0.22          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 10       | 0.22          |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB2  | 7        | 0.22          |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB3  | 7        | 0.22          |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB2  | 7        | 0.22          |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB3  | 7        | 0.22          |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB2  | 7        | 0.22          |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB3  | 7        | 0.22          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD11  | 12       | 0.22          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD12  | 12       | 0.22          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD13  | 12       | 0.22          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD11  | 12       | 0.22          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD12  | 12       | 0.22          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD13  | 12       | 0.22          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD11  | 12       | 0.22          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD12  | 12       | 0.22          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD13  | 12       | 0.22          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG11  | 10       | 0.22          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG12  | 10       | 0.22          |
| (1,1239) | 1:49:A:MET:HB2   | 1:53:A:VAL:HG13  | 10       | 0.22          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG11  | 10       | 0.22          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG12  | 10       | 0.22          |
| (1,1239) | 1:49:A:MET:HB3   | 1:53:A:VAL:HG13  | 10       | 0.22          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG21  | 7        | 0.22          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG22  | 7        | 0.22          |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG23  | 7        | 0.22          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11  | 2        | 0.22          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,810) | 1:33:A:THR:H     | 1:32:A:VAL:HG12 | 2        | 0.22          |
| (1,810) | 1:33:A:THR:H     | 1:32:A:VAL:HG13 | 2        | 0.22          |
| (1,810) | 1:33:A:THR:H     | 1:32:A:VAL:HG11 | 18       | 0.22          |
| (1,810) | 1:33:A:THR:H     | 1:32:A:VAL:HG12 | 18       | 0.22          |
| (1,810) | 1:33:A:THR:H     | 1:32:A:VAL:HG13 | 18       | 0.22          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB2  | 3        | 0.22          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB3  | 3        | 0.22          |
| (1,405) | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB  | 20       | 0.22          |
| (1,405) | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB  | 20       | 0.22          |
| (1,405) | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB  | 20       | 0.22          |
| (1,318) | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG21  | 12       | 0.22          |
| (1,318) | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG22  | 12       | 0.22          |
| (1,318) | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG23  | 12       | 0.22          |
| (1,318) | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG21  | 12       | 0.22          |
| (1,318) | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG22  | 12       | 0.22          |
| (1,318) | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG23  | 12       | 0.22          |
| (1,318) | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG21  | 12       | 0.22          |
| (1,318) | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG22  | 12       | 0.22          |
| (1,318) | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG23  | 12       | 0.22          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG21  | 2        | 0.22          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG22  | 2        | 0.22          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG23  | 2        | 0.22          |
| (1,259) | 1:75:A:VAL:HB    | 1:4:A:VAL:HG11  | 15       | 0.22          |
| (1,259) | 1:75:A:VAL:HB    | 1:4:A:VAL:HG12  | 15       | 0.22          |
| (1,259) | 1:75:A:VAL:HB    | 1:4:A:VAL:HG13  | 15       | 0.22          |
| (1,145) | 1:32:A:VAL:HG21  | 1:6:A:PHE:HZ    | 19       | 0.22          |
| (1,145) | 1:32:A:VAL:HG22  | 1:6:A:PHE:HZ    | 19       | 0.22          |
| (1,145) | 1:32:A:VAL:HG23  | 1:6:A:PHE:HZ    | 19       | 0.22          |
| (1,87)  | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD1 | 8        | 0.22          |
| (1,87)  | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD2 | 8        | 0.22          |
| (1,87)  | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD1 | 8        | 0.22          |
| (1,87)  | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD2 | 8        | 0.22          |
| (1,87)  | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD1 | 8        | 0.22          |
| (1,87)  | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD2 | 8        | 0.22          |
| (1,44)  | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2  | 4        | 0.22          |
| (1,44)  | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3  | 4        | 0.22          |
| (1,44)  | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2  | 4        | 0.22          |
| (1,44)  | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3  | 4        | 0.22          |
| (1,44)  | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2  | 4        | 0.22          |
| (1,44)  | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3  | 4        | 0.22          |
| (1,44)  | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2  | 9        | 0.22          |
| (1,44)  | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3  | 9        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2   | 9        | 0.22          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3   | 9        | 0.22          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2   | 9        | 0.22          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3   | 9        | 0.22          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H    | 11       | 0.21          |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H    | 11       | 0.21          |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H    | 11       | 0.21          |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG11 | 1        | 0.21          |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG12 | 1        | 0.21          |
| (1,2762) | 1:21:A:PHE:HB2   | 1:119:A:VAL:HG13 | 1        | 0.21          |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG11 | 1        | 0.21          |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG12 | 1        | 0.21          |
| (1,2762) | 1:21:A:PHE:HB3   | 1:119:A:VAL:HG13 | 1        | 0.21          |
| (1,2746) | 1:119:A:VAL:HG21 | 1:15:A:SER:HA    | 4        | 0.21          |
| (1,2746) | 1:119:A:VAL:HG22 | 1:15:A:SER:HA    | 4        | 0.21          |
| (1,2746) | 1:119:A:VAL:HG23 | 1:15:A:SER:HA    | 4        | 0.21          |
| (1,2653) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HB   | 7        | 0.21          |
| (1,2653) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HB   | 7        | 0.21          |
| (1,2653) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HB   | 7        | 0.21          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG21 | 4        | 0.21          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG22 | 4        | 0.21          |
| (1,2431) | 1:122:A:ARG:HD2  | 1:119:A:VAL:HG23 | 4        | 0.21          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG21 | 4        | 0.21          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG22 | 4        | 0.21          |
| (1,2431) | 1:122:A:ARG:HD3  | 1:119:A:VAL:HG23 | 4        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 5        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 5        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 5        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 5        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 5        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 5        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 6        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 6        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 6        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 6        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 6        | 0.21          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 6        | 0.21          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 1        | 0.21          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 1        | 0.21          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 2        | 0.21          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 2        | 0.21          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 2        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 2        | 0.21          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 2        | 0.21          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 2        | 0.21          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 2        | 0.21          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 2        | 0.21          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 2        | 0.21          |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG21 | 5        | 0.21          |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG22 | 5        | 0.21          |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG23 | 5        | 0.21          |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG21 | 5        | 0.21          |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG22 | 5        | 0.21          |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG23 | 5        | 0.21          |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG21 | 19       | 0.21          |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG22 | 19       | 0.21          |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG23 | 19       | 0.21          |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG21 | 19       | 0.21          |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG22 | 19       | 0.21          |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG23 | 19       | 0.21          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD21 | 15       | 0.21          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD22 | 15       | 0.21          |
| (1,2207) | 1:109:A:LEU:HA   | 1:109:A:LEU:HD23 | 15       | 0.21          |
| (1,2176) | 1:109:A:LEU:HD21 | 1:108:A:SER:HA   | 14       | 0.21          |
| (1,2176) | 1:109:A:LEU:HD22 | 1:108:A:SER:HA   | 14       | 0.21          |
| (1,2176) | 1:109:A:LEU:HD23 | 1:108:A:SER:HA   | 14       | 0.21          |
| (1,845)  | 1:79:A:LEU:HD11  | 1:34:A:SER:HA    | 17       | 0.21          |
| (1,845)  | 1:79:A:LEU:HD12  | 1:34:A:SER:HA    | 17       | 0.21          |
| (1,845)  | 1:79:A:LEU:HD13  | 1:34:A:SER:HA    | 17       | 0.21          |
| (1,826)  | 1:5:A:MET:HA     | 1:33:A:THR:HA    | 13       | 0.21          |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG2   | 18       | 0.21          |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG3   | 18       | 0.21          |
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG2   | 18       | 0.21          |
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG3   | 18       | 0.21          |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG2   | 18       | 0.21          |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG3   | 18       | 0.21          |
| (1,448)  | 1:19:A:GLU:H     | 1:16:A:GLN:HB2   | 11       | 0.21          |
| (1,448)  | 1:19:A:GLU:H     | 1:16:A:GLN:HB3   | 11       | 0.21          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2   | 7        | 0.21          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3   | 7        | 0.21          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2   | 7        | 0.21          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3   | 7        | 0.21          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2   | 10       | 0.21          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3   | 10       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2   | 10       | 0.21          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3   | 10       | 0.21          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG21   | 12       | 0.21          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG22   | 12       | 0.21          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG23   | 12       | 0.21          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG21   | 19       | 0.21          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG22   | 19       | 0.21          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG23   | 19       | 0.21          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2   | 8        | 0.21          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3   | 8        | 0.21          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2   | 8        | 0.21          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3   | 8        | 0.21          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2   | 8        | 0.21          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3   | 8        | 0.21          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD11  | 1        | 0.21          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD12  | 1        | 0.21          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD13  | 1        | 0.21          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 1        | 0.2           |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 1        | 0.2           |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 1        | 0.2           |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 19       | 0.2           |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 19       | 0.2           |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 19       | 0.2           |
| (1,3559) | 1:111:A:VAL:HG21 | 1:115:A:VAL:H    | 5        | 0.2           |
| (1,3559) | 1:111:A:VAL:HG22 | 1:115:A:VAL:H    | 5        | 0.2           |
| (1,3559) | 1:111:A:VAL:HG23 | 1:115:A:VAL:H    | 5        | 0.2           |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H    | 15       | 0.2           |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H    | 15       | 0.2           |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H    | 15       | 0.2           |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H    | 19       | 0.2           |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H    | 19       | 0.2           |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H    | 19       | 0.2           |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H     | 11       | 0.2           |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H     | 11       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 4        | 0.2           |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 4        | 0.2           |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 4        | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 4        | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 4        | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 4        | 0.2           |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 8        | 0.2           |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 8        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 8        | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 8        | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 8        | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 8        | 0.2           |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 14       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 14       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 14       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 14       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 14       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 14       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 16       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 16       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 16       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 16       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 16       | 0.2           |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 16       | 0.2           |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 3        | 0.2           |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 3        | 0.2           |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 14       | 0.2           |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 14       | 0.2           |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG21 | 5        | 0.2           |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG22 | 5        | 0.2           |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG23 | 5        | 0.2           |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG21 | 20       | 0.2           |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG22 | 20       | 0.2           |
| (1,2245) | 1:104:A:PRO:HB2  | 1:111:A:VAL:HG23 | 20       | 0.2           |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG21 | 20       | 0.2           |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG22 | 20       | 0.2           |
| (1,2245) | 1:104:A:PRO:HB3  | 1:111:A:VAL:HG23 | 20       | 0.2           |
| (1,2176) | 1:109:A:LEU:HD21 | 1:108:A:SER:HA   | 10       | 0.2           |
| (1,2176) | 1:109:A:LEU:HD22 | 1:108:A:SER:HA   | 10       | 0.2           |
| (1,2176) | 1:109:A:LEU:HD23 | 1:108:A:SER:HA   | 10       | 0.2           |
| (1,2176) | 1:109:A:LEU:HD21 | 1:108:A:SER:HA   | 16       | 0.2           |
| (1,2176) | 1:109:A:LEU:HD22 | 1:108:A:SER:HA   | 16       | 0.2           |
| (1,2176) | 1:109:A:LEU:HD23 | 1:108:A:SER:HA   | 16       | 0.2           |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG21  | 14       | 0.2           |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG22  | 14       | 0.2           |
| (1,821)  | 1:33:A:THR:H     | 1:32:A:VAL:HG23  | 14       | 0.2           |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11  | 1        | 0.2           |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG12  | 1        | 0.2           |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG13  | 1        | 0.2           |
| (1,793)  | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB    | 17       | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,793) | 1:31:A:ALA:HB2  | 1:32:A:VAL:HB   | 17       | 0.2           |
| (1,793) | 1:31:A:ALA:HB3  | 1:32:A:VAL:HB   | 17       | 0.2           |
| (1,633) | 1:62:A:SER:HA   | 1:61:A:THR:HB   | 2        | 0.2           |
| (1,633) | 1:62:A:SER:HA   | 1:61:A:THR:HB   | 14       | 0.2           |
| (1,448) | 1:19:A:GLU:H    | 1:16:A:GLN:HB2  | 18       | 0.2           |
| (1,448) | 1:19:A:GLU:H    | 1:16:A:GLN:HB3  | 18       | 0.2           |
| (1,446) | 1:62:A:SER:HA   | 1:16:A:GLN:HB2  | 9        | 0.2           |
| (1,446) | 1:62:A:SER:HA   | 1:16:A:GLN:HB3  | 9        | 0.2           |
| (1,443) | 1:10:A:ARG:HB2  | 1:16:A:GLN:HB2  | 15       | 0.2           |
| (1,443) | 1:10:A:ARG:HB2  | 1:16:A:GLN:HB3  | 15       | 0.2           |
| (1,443) | 1:10:A:ARG:HB3  | 1:16:A:GLN:HB2  | 15       | 0.2           |
| (1,443) | 1:10:A:ARG:HB3  | 1:16:A:GLN:HB3  | 15       | 0.2           |
| (1,340) | 1:104:A:PRO:HD2 | 1:8:A:SER:HB2   | 10       | 0.2           |
| (1,340) | 1:104:A:PRO:HD2 | 1:8:A:SER:HB3   | 10       | 0.2           |
| (1,340) | 1:104:A:PRO:HD3 | 1:8:A:SER:HB2   | 10       | 0.2           |
| (1,340) | 1:104:A:PRO:HD3 | 1:8:A:SER:HB3   | 10       | 0.2           |
| (1,340) | 1:104:A:PRO:HD2 | 1:8:A:SER:HB2   | 16       | 0.2           |
| (1,340) | 1:104:A:PRO:HD2 | 1:8:A:SER:HB3   | 16       | 0.2           |
| (1,340) | 1:104:A:PRO:HD3 | 1:8:A:SER:HB2   | 16       | 0.2           |
| (1,340) | 1:104:A:PRO:HD3 | 1:8:A:SER:HB3   | 16       | 0.2           |
| (1,259) | 1:75:A:VAL:HB   | 1:4:A:VAL:HG11  | 9        | 0.2           |
| (1,259) | 1:75:A:VAL:HB   | 1:4:A:VAL:HG12  | 9        | 0.2           |
| (1,259) | 1:75:A:VAL:HB   | 1:4:A:VAL:HG13  | 9        | 0.2           |
| (1,49)  | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG2  | 6        | 0.2           |
| (1,49)  | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG3  | 6        | 0.2           |
| (1,49)  | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG2  | 6        | 0.2           |
| (1,49)  | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG3  | 6        | 0.2           |
| (1,49)  | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG2  | 6        | 0.2           |
| (1,49)  | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG3  | 6        | 0.2           |
| (1,47)  | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG2  | 6        | 0.2           |
| (1,47)  | 1:37:A:LEU:HD11 | 1:87:A:PRO:HG3  | 6        | 0.2           |
| (1,47)  | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG2  | 6        | 0.2           |
| (1,47)  | 1:37:A:LEU:HD12 | 1:87:A:PRO:HG3  | 6        | 0.2           |
| (1,47)  | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG2  | 6        | 0.2           |
| (1,47)  | 1:37:A:LEU:HD13 | 1:87:A:PRO:HG3  | 6        | 0.2           |
| (1,44)  | 1:86:A:LEU:HD11 | 1:87:A:PRO:HB2  | 6        | 0.2           |
| (1,44)  | 1:86:A:LEU:HD11 | 1:87:A:PRO:HB3  | 6        | 0.2           |
| (1,44)  | 1:86:A:LEU:HD12 | 1:87:A:PRO:HB2  | 6        | 0.2           |
| (1,44)  | 1:86:A:LEU:HD12 | 1:87:A:PRO:HB3  | 6        | 0.2           |
| (1,44)  | 1:86:A:LEU:HD13 | 1:87:A:PRO:HB2  | 6        | 0.2           |
| (1,44)  | 1:86:A:LEU:HD13 | 1:87:A:PRO:HB3  | 6        | 0.2           |
| (1,40)  | 1:91:A:VAL:H    | 1:86:A:LEU:HD11 | 13       | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD12  | 13       | 0.2           |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD13  | 13       | 0.2           |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 4        | 0.19          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 4        | 0.19          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 4        | 0.19          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H     | 9        | 0.19          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H     | 9        | 0.19          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H     | 12       | 0.19          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H     | 12       | 0.19          |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H     | 17       | 0.19          |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H     | 17       | 0.19          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2   | 17       | 0.19          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3   | 17       | 0.19          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2   | 17       | 0.19          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3   | 17       | 0.19          |
| (1,2653) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HB   | 11       | 0.19          |
| (1,2653) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HB   | 11       | 0.19          |
| (1,2653) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HB   | 11       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 7        | 0.19          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 7        | 0.19          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 7        | 0.19          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 7        | 0.19          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 7        | 0.19          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 7        | 0.19          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 15       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 15       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 15       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 15       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 15       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 15       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 17       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 17       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 17       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 17       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 17       | 0.19          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 17       | 0.19          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 4        | 0.19          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 4        | 0.19          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 5        | 0.19          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 5        | 0.19          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 12       | 0.19          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 12       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 17       | 0.19          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 17       | 0.19          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 18       | 0.19          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 18       | 0.19          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 3        | 0.19          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 3        | 0.19          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 3        | 0.19          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 3        | 0.19          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 3        | 0.19          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 3        | 0.19          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 3        | 0.19          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 3        | 0.19          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 3        | 0.19          |
| (1,2022) | 1:100:A:GLN:H    | 1:98:A:ASP:HA    | 10       | 0.19          |
| (1,2022) | 1:100:A:GLN:H    | 1:98:A:ASP:HA    | 13       | 0.19          |
| (1,1813) | 1:86:A:LEU:HA    | 1:86:A:LEU:HD21  | 17       | 0.19          |
| (1,1813) | 1:86:A:LEU:HA    | 1:86:A:LEU:HD22  | 17       | 0.19          |
| (1,1813) | 1:86:A:LEU:HA    | 1:86:A:LEU:HD23  | 17       | 0.19          |
| (1,1777) | 1:86:A:LEU:HD21  | 1:86:A:LEU:HA    | 17       | 0.19          |
| (1,1777) | 1:86:A:LEU:HD22  | 1:86:A:LEU:HA    | 17       | 0.19          |
| (1,1777) | 1:86:A:LEU:HD23  | 1:86:A:LEU:HA    | 17       | 0.19          |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB2   | 17       | 0.19          |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB3   | 17       | 0.19          |
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB2   | 17       | 0.19          |
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB3   | 17       | 0.19          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21  | 9        | 0.19          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22  | 9        | 0.19          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23  | 9        | 0.19          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21  | 14       | 0.19          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22  | 14       | 0.19          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23  | 14       | 0.19          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD11  | 13       | 0.19          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD12  | 13       | 0.19          |
| (1,910)  | 1:65:A:ILE:HD11  | 1:37:A:LEU:HD13  | 13       | 0.19          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD11  | 13       | 0.19          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD12  | 13       | 0.19          |
| (1,910)  | 1:65:A:ILE:HD12  | 1:37:A:LEU:HD13  | 13       | 0.19          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD11  | 13       | 0.19          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD12  | 13       | 0.19          |
| (1,910)  | 1:65:A:ILE:HD13  | 1:37:A:LEU:HD13  | 13       | 0.19          |
| (1,826)  | 1:5:A:MET:HA     | 1:33:A:THR:HA    | 8        | 0.19          |
| (1,826)  | 1:5:A:MET:HA     | 1:33:A:THR:HA    | 15       | 0.19          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG21 | 3        | 0.19          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG22 | 3        | 0.19          |
| (1,821) | 1:33:A:THR:H     | 1:32:A:VAL:HG23 | 3        | 0.19          |
| (1,793) | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB   | 7        | 0.19          |
| (1,793) | 1:31:A:ALA:HB2   | 1:32:A:VAL:HB   | 7        | 0.19          |
| (1,793) | 1:31:A:ALA:HB3   | 1:32:A:VAL:HB   | 7        | 0.19          |
| (1,793) | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB   | 10       | 0.19          |
| (1,793) | 1:31:A:ALA:HB2   | 1:32:A:VAL:HB   | 10       | 0.19          |
| (1,793) | 1:31:A:ALA:HB3   | 1:32:A:VAL:HB   | 10       | 0.19          |
| (1,633) | 1:62:A:SER:HA    | 1:61:A:THR:HB   | 9        | 0.19          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB2  | 14       | 0.19          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB3  | 14       | 0.19          |
| (1,443) | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2  | 20       | 0.19          |
| (1,443) | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3  | 20       | 0.19          |
| (1,443) | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2  | 20       | 0.19          |
| (1,443) | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3  | 20       | 0.19          |
| (1,405) | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB  | 4        | 0.19          |
| (1,405) | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB  | 4        | 0.19          |
| (1,405) | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB  | 4        | 0.19          |
| (1,405) | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB  | 8        | 0.19          |
| (1,405) | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB  | 8        | 0.19          |
| (1,405) | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB  | 8        | 0.19          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG11  | 1        | 0.19          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG12  | 1        | 0.19          |
| (1,261) | 1:126:A:LEU:HD21 | 1:4:A:VAL:HG13  | 1        | 0.19          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG11  | 1        | 0.19          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG12  | 1        | 0.19          |
| (1,261) | 1:126:A:LEU:HD22 | 1:4:A:VAL:HG13  | 1        | 0.19          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG11  | 1        | 0.19          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG12  | 1        | 0.19          |
| (1,261) | 1:126:A:LEU:HD23 | 1:4:A:VAL:HG13  | 1        | 0.19          |
| (1,139) | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1   | 1        | 0.19          |
| (1,139) | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2   | 1        | 0.19          |
| (1,44)  | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2  | 3        | 0.19          |
| (1,44)  | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3  | 3        | 0.19          |
| (1,44)  | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2  | 3        | 0.19          |
| (1,44)  | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3  | 3        | 0.19          |
| (1,44)  | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2  | 3        | 0.19          |
| (1,44)  | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3  | 3        | 0.19          |
| (1,40)  | 1:91:A:VAL:H     | 1:86:A:LEU:HD11 | 10       | 0.19          |
| (1,40)  | 1:91:A:VAL:H     | 1:86:A:LEU:HD12 | 10       | 0.19          |
| (1,40)  | 1:91:A:VAL:H     | 1:86:A:LEU:HD13 | 10       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H    | 13       | 0.18          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H    | 13       | 0.18          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H    | 13       | 0.18          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H    | 20       | 0.18          |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H    | 20       | 0.18          |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H    | 20       | 0.18          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H     | 5        | 0.18          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H     | 5        | 0.18          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H     | 6        | 0.18          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H     | 6        | 0.18          |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H     | 8        | 0.18          |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H     | 8        | 0.18          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG11 | 16       | 0.18          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG12 | 16       | 0.18          |
| (1,2565) | 1:18:A:ALA:HA    | 1:123:A:VAL:HG13 | 16       | 0.18          |
| (1,2434) | 1:79:A:LEU:HD21  | 1:119:A:VAL:HG21 | 19       | 0.18          |
| (1,2434) | 1:79:A:LEU:HD21  | 1:119:A:VAL:HG22 | 19       | 0.18          |
| (1,2434) | 1:79:A:LEU:HD21  | 1:119:A:VAL:HG23 | 19       | 0.18          |
| (1,2434) | 1:79:A:LEU:HD22  | 1:119:A:VAL:HG21 | 19       | 0.18          |
| (1,2434) | 1:79:A:LEU:HD22  | 1:119:A:VAL:HG22 | 19       | 0.18          |
| (1,2434) | 1:79:A:LEU:HD22  | 1:119:A:VAL:HG23 | 19       | 0.18          |
| (1,2434) | 1:79:A:LEU:HD23  | 1:119:A:VAL:HG21 | 19       | 0.18          |
| (1,2434) | 1:79:A:LEU:HD23  | 1:119:A:VAL:HG22 | 19       | 0.18          |
| (1,2434) | 1:79:A:LEU:HD23  | 1:119:A:VAL:HG23 | 19       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 12       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 12       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 12       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 12       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 12       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 12       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 18       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 18       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 18       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 18       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 18       | 0.18          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 18       | 0.18          |
| (1,2351) | 1:114:A:THR:H    | 1:116:A:ARG:HG2  | 10       | 0.18          |
| (1,2351) | 1:114:A:THR:H    | 1:116:A:ARG:HG3  | 10       | 0.18          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 7        | 0.18          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 7        | 0.18          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 7        | 0.18          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 7        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 7        | 0.18          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 7        | 0.18          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 7        | 0.18          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 7        | 0.18          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 7        | 0.18          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 12       | 0.18          |
| (1,2119) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 12       | 0.18          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 12       | 0.18          |
| (1,2119) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 12       | 0.18          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 12       | 0.18          |
| (1,2119) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 12       | 0.18          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB2  | 12       | 0.18          |
| (1,2111) | 1:111:A:VAL:HG21 | 1:104:A:PRO:HB3  | 12       | 0.18          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB2  | 12       | 0.18          |
| (1,2111) | 1:111:A:VAL:HG22 | 1:104:A:PRO:HB3  | 12       | 0.18          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB2  | 12       | 0.18          |
| (1,2111) | 1:111:A:VAL:HG23 | 1:104:A:PRO:HB3  | 12       | 0.18          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG11  | 9        | 0.18          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG12  | 9        | 0.18          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG13  | 9        | 0.18          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG11  | 9        | 0.18          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG12  | 9        | 0.18          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG13  | 9        | 0.18          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG11  | 9        | 0.18          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG12  | 9        | 0.18          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG13  | 9        | 0.18          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG11  | 17       | 0.18          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG12  | 17       | 0.18          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG13  | 17       | 0.18          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG11  | 17       | 0.18          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG12  | 17       | 0.18          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG13  | 17       | 0.18          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG11  | 17       | 0.18          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG12  | 17       | 0.18          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG13  | 17       | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21  | 7        | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22  | 7        | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23  | 7        | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21  | 11       | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22  | 11       | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23  | 11       | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21  | 13       | 0.18          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22 | 13       | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23 | 13       | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21 | 16       | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22 | 16       | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23 | 16       | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21 | 20       | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22 | 20       | 0.18          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23 | 20       | 0.18          |
| (1,991)  | 1:57:A:ILE:H     | 1:42:A:VAL:HB   | 17       | 0.18          |
| (1,991)  | 1:57:A:ILE:H     | 1:42:A:VAL:HB   | 20       | 0.18          |
| (1,928)  | 1:40:A:SER:HA    | 1:38:A:GLU:HA   | 20       | 0.18          |
| (1,845)  | 1:79:A:LEU:HD11  | 1:34:A:SER:HA   | 5        | 0.18          |
| (1,845)  | 1:79:A:LEU:HD12  | 1:34:A:SER:HA   | 5        | 0.18          |
| (1,845)  | 1:79:A:LEU:HD13  | 1:34:A:SER:HA   | 5        | 0.18          |
| (1,793)  | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB   | 16       | 0.18          |
| (1,793)  | 1:31:A:ALA:HB2   | 1:32:A:VAL:HB   | 16       | 0.18          |
| (1,793)  | 1:31:A:ALA:HB3   | 1:32:A:VAL:HB   | 16       | 0.18          |
| (1,793)  | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB   | 20       | 0.18          |
| (1,793)  | 1:31:A:ALA:HB2   | 1:32:A:VAL:HB   | 20       | 0.18          |
| (1,793)  | 1:31:A:ALA:HB3   | 1:32:A:VAL:HB   | 20       | 0.18          |
| (1,633)  | 1:62:A:SER:HA    | 1:61:A:THR:HB   | 16       | 0.18          |
| (1,483)  | 1:123:A:VAL:HG11 | 1:18:A:ALA:HA   | 16       | 0.18          |
| (1,483)  | 1:123:A:VAL:HG12 | 1:18:A:ALA:HA   | 16       | 0.18          |
| (1,483)  | 1:123:A:VAL:HG13 | 1:18:A:ALA:HA   | 16       | 0.18          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2  | 3        | 0.18          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3  | 3        | 0.18          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2  | 3        | 0.18          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3  | 3        | 0.18          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2  | 6        | 0.18          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3  | 6        | 0.18          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2  | 6        | 0.18          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3  | 6        | 0.18          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG11  | 10       | 0.18          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG12  | 10       | 0.18          |
| (1,259)  | 1:75:A:VAL:HB    | 1:4:A:VAL:HG13  | 10       | 0.18          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG11  | 6        | 0.18          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG12  | 6        | 0.18          |
| (1,256)  | 1:3:A:LYS:HA     | 1:4:A:VAL:HG13  | 6        | 0.18          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1   | 16       | 0.18          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2   | 16       | 0.18          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H   | 2        | 0.17          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H   | 2        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 2        | 0.17          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 5        | 0.17          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 5        | 0.17          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 5        | 0.17          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H    | 6        | 0.17          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H    | 6        | 0.17          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H    | 6        | 0.17          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H    | 15       | 0.17          |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H     | 9        | 0.17          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H     | 3        | 0.17          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H     | 3        | 0.17          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H     | 8        | 0.17          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H     | 8        | 0.17          |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H     | 4        | 0.17          |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H     | 4        | 0.17          |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H     | 12       | 0.17          |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H     | 12       | 0.17          |
| (1,2772) | 1:4:A:VAL:HG21   | 1:77:A:ILE:HG12  | 5        | 0.17          |
| (1,2772) | 1:4:A:VAL:HG21   | 1:77:A:ILE:HG13  | 5        | 0.17          |
| (1,2772) | 1:4:A:VAL:HG22   | 1:77:A:ILE:HG12  | 5        | 0.17          |
| (1,2772) | 1:4:A:VAL:HG22   | 1:77:A:ILE:HG13  | 5        | 0.17          |
| (1,2772) | 1:4:A:VAL:HG23   | 1:77:A:ILE:HG12  | 5        | 0.17          |
| (1,2772) | 1:4:A:VAL:HG23   | 1:77:A:ILE:HG13  | 5        | 0.17          |
| (1,2649) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HA   | 11       | 0.17          |
| (1,2649) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HA   | 11       | 0.17          |
| (1,2649) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HA   | 11       | 0.17          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD11 | 10       | 0.17          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD12 | 10       | 0.17          |
| (1,2416) | 1:6:A:PHE:HD1    | 1:126:A:LEU:HD13 | 10       | 0.17          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD11 | 10       | 0.17          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD12 | 10       | 0.17          |
| (1,2416) | 1:6:A:PHE:HD2    | 1:126:A:LEU:HD13 | 10       | 0.17          |
| (1,2405) | 1:119:A:VAL:H    | 1:119:A:VAL:HB   | 19       | 0.17          |
| (1,2405) | 1:119:A:VAL:H    | 1:119:A:VAL:HB   | 20       | 0.17          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 2        | 0.17          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 2        | 0.17          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 7        | 0.17          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 7        | 0.17          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 8        | 0.17          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 8        | 0.17          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 10       | 0.17          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 10       | 0.17          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA  | 13       | 0.17          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA  | 13       | 0.17          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA  | 15       | 0.17          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA  | 15       | 0.17          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA  | 19       | 0.17          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA  | 19       | 0.17          |
| (1,2351) | 1:114:A:THR:H    | 1:116:A:ARG:HG2 | 3        | 0.17          |
| (1,2351) | 1:114:A:THR:H    | 1:116:A:ARG:HG3 | 3        | 0.17          |
| (1,2124) | 1:4:A:VAL:HG21   | 1:126:A:LEU:HG  | 4        | 0.17          |
| (1,2124) | 1:4:A:VAL:HG22   | 1:126:A:LEU:HG  | 4        | 0.17          |
| (1,2124) | 1:4:A:VAL:HG23   | 1:126:A:LEU:HG  | 4        | 0.17          |
| (1,2124) | 1:4:A:VAL:HG21   | 1:126:A:LEU:HG  | 12       | 0.17          |
| (1,2124) | 1:4:A:VAL:HG22   | 1:126:A:LEU:HG  | 12       | 0.17          |
| (1,2124) | 1:4:A:VAL:HG23   | 1:126:A:LEU:HG  | 12       | 0.17          |
| (1,1776) | 1:37:A:LEU:HD11  | 1:86:A:LEU:HA   | 10       | 0.17          |
| (1,1776) | 1:37:A:LEU:HD12  | 1:86:A:LEU:HA   | 10       | 0.17          |
| (1,1776) | 1:37:A:LEU:HD13  | 1:86:A:LEU:HA   | 10       | 0.17          |
| (1,1756) | 1:86:A:LEU:HD11  | 1:84:A:VAL:HA   | 8        | 0.17          |
| (1,1756) | 1:86:A:LEU:HD12  | 1:84:A:VAL:HA   | 8        | 0.17          |
| (1,1756) | 1:86:A:LEU:HD13  | 1:84:A:VAL:HA   | 8        | 0.17          |
| (1,1734) | 1:119:A:VAL:HG21 | 1:79:A:LEU:HD11 | 20       | 0.17          |
| (1,1734) | 1:119:A:VAL:HG21 | 1:79:A:LEU:HD12 | 20       | 0.17          |
| (1,1734) | 1:119:A:VAL:HG21 | 1:79:A:LEU:HD13 | 20       | 0.17          |
| (1,1734) | 1:119:A:VAL:HG22 | 1:79:A:LEU:HD11 | 20       | 0.17          |
| (1,1734) | 1:119:A:VAL:HG22 | 1:79:A:LEU:HD12 | 20       | 0.17          |
| (1,1734) | 1:119:A:VAL:HG22 | 1:79:A:LEU:HD13 | 20       | 0.17          |
| (1,1734) | 1:119:A:VAL:HG23 | 1:79:A:LEU:HD11 | 20       | 0.17          |
| (1,1734) | 1:119:A:VAL:HG23 | 1:79:A:LEU:HD12 | 20       | 0.17          |
| (1,1734) | 1:119:A:VAL:HG23 | 1:79:A:LEU:HD13 | 20       | 0.17          |
| (1,1730) | 1:99:A:TRP:H     | 1:79:A:LEU:HG   | 16       | 0.17          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG11 | 6        | 0.17          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG12 | 6        | 0.17          |
| (1,1600) | 1:76:A:VAL:HG21  | 1:75:A:VAL:HG13 | 6        | 0.17          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG11 | 6        | 0.17          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG12 | 6        | 0.17          |
| (1,1600) | 1:76:A:VAL:HG22  | 1:75:A:VAL:HG13 | 6        | 0.17          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG11 | 6        | 0.17          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG12 | 6        | 0.17          |
| (1,1600) | 1:76:A:VAL:HG23  | 1:75:A:VAL:HG13 | 6        | 0.17          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21 | 2        | 0.17          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22 | 2        | 0.17          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23 | 2        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21  | 3        | 0.17          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22  | 3        | 0.17          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23  | 3        | 0.17          |
| (1,991)  | 1:57:A:ILE:H     | 1:42:A:VAL:HB    | 5        | 0.17          |
| (1,991)  | 1:57:A:ILE:H     | 1:42:A:VAL:HB    | 13       | 0.17          |
| (1,928)  | 1:40:A:SER:HA    | 1:38:A:GLU:HA    | 17       | 0.17          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD11  | 10       | 0.17          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD12  | 10       | 0.17          |
| (1,917)  | 1:86:A:LEU:HA    | 1:37:A:LEU:HD13  | 10       | 0.17          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG21 | 16       | 0.17          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG22 | 16       | 0.17          |
| (1,814)  | 1:25:A:LEU:HB2   | 1:123:A:VAL:HG23 | 16       | 0.17          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG21 | 16       | 0.17          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG22 | 16       | 0.17          |
| (1,814)  | 1:25:A:LEU:HB3   | 1:123:A:VAL:HG23 | 16       | 0.17          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG11  | 4        | 0.17          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG12  | 4        | 0.17          |
| (1,810)  | 1:33:A:THR:H     | 1:32:A:VAL:HG13  | 4        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB    | 2        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB2   | 1:32:A:VAL:HB    | 2        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB3   | 1:32:A:VAL:HB    | 2        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB    | 3        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB2   | 1:32:A:VAL:HB    | 3        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB3   | 1:32:A:VAL:HB    | 3        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB    | 6        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB2   | 1:32:A:VAL:HB    | 6        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB3   | 1:32:A:VAL:HB    | 6        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB    | 9        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB2   | 1:32:A:VAL:HB    | 9        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB3   | 1:32:A:VAL:HB    | 9        | 0.17          |
| (1,793)  | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB    | 14       | 0.17          |
| (1,793)  | 1:31:A:ALA:HB2   | 1:32:A:VAL:HB    | 14       | 0.17          |
| (1,793)  | 1:31:A:ALA:HB3   | 1:32:A:VAL:HB    | 14       | 0.17          |
| (1,633)  | 1:62:A:SER:HA    | 1:61:A:THR:HB    | 4        | 0.17          |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG2   | 8        | 0.17          |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG3   | 8        | 0.17          |
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG2   | 8        | 0.17          |
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG3   | 8        | 0.17          |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG2   | 8        | 0.17          |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG3   | 8        | 0.17          |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG2   | 15       | 0.17          |
| (1,480)  | 1:119:A:VAL:HG11 | 1:17:A:MET:HG3   | 15       | 0.17          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG2  | 15       | 0.17          |
| (1,480)  | 1:119:A:VAL:HG12 | 1:17:A:MET:HG3  | 15       | 0.17          |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG2  | 15       | 0.17          |
| (1,480)  | 1:119:A:VAL:HG13 | 1:17:A:MET:HG3  | 15       | 0.17          |
| (1,448)  | 1:19:A:GLU:H     | 1:16:A:GLN:HB2  | 2        | 0.17          |
| (1,448)  | 1:19:A:GLU:H     | 1:16:A:GLN:HB3  | 2        | 0.17          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2  | 12       | 0.17          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3  | 12       | 0.17          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2  | 12       | 0.17          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3  | 12       | 0.17          |
| (1,433)  | 1:50:A:MET:HE1   | 1:16:A:GLN:HA   | 8        | 0.17          |
| (1,433)  | 1:50:A:MET:HE2   | 1:16:A:GLN:HA   | 8        | 0.17          |
| (1,433)  | 1:50:A:MET:HE3   | 1:16:A:GLN:HA   | 8        | 0.17          |
| (1,433)  | 1:50:A:MET:HE1   | 1:16:A:GLN:HA   | 18       | 0.17          |
| (1,433)  | 1:50:A:MET:HE2   | 1:16:A:GLN:HA   | 18       | 0.17          |
| (1,433)  | 1:50:A:MET:HE3   | 1:16:A:GLN:HA   | 18       | 0.17          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG21  | 10       | 0.17          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG22  | 10       | 0.17          |
| (1,267)  | 1:76:A:VAL:HA    | 1:4:A:VAL:HG23  | 10       | 0.17          |
| (1,263)  | 1:77:A:ILE:HG12  | 1:4:A:VAL:HG21  | 5        | 0.17          |
| (1,263)  | 1:77:A:ILE:HG12  | 1:4:A:VAL:HG22  | 5        | 0.17          |
| (1,263)  | 1:77:A:ILE:HG12  | 1:4:A:VAL:HG23  | 5        | 0.17          |
| (1,263)  | 1:77:A:ILE:HG13  | 1:4:A:VAL:HG21  | 5        | 0.17          |
| (1,263)  | 1:77:A:ILE:HG13  | 1:4:A:VAL:HG22  | 5        | 0.17          |
| (1,263)  | 1:77:A:ILE:HG13  | 1:4:A:VAL:HG23  | 5        | 0.17          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1   | 5        | 0.17          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2   | 5        | 0.17          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1   | 20       | 0.17          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2   | 20       | 0.17          |
| (1,87)   | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD1 | 7        | 0.17          |
| (1,87)   | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD2 | 7        | 0.17          |
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD1 | 7        | 0.17          |
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD2 | 7        | 0.17          |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD1 | 7        | 0.17          |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD2 | 7        | 0.17          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2  | 18       | 0.17          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3  | 18       | 0.17          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2  | 18       | 0.17          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3  | 18       | 0.17          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2  | 18       | 0.17          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3  | 18       | 0.17          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1  | 19       | 0.16          |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1 | 19       | 0.16          |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1 | 19       | 0.16          |
| (1,3602) | 1:25:A:LEU:HD11  | 1:121:A:GLU:H  | 8        | 0.16          |
| (1,3602) | 1:25:A:LEU:HD12  | 1:121:A:GLU:H  | 8        | 0.16          |
| (1,3602) | 1:25:A:LEU:HD13  | 1:121:A:GLU:H  | 8        | 0.16          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 1        | 0.16          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 4        | 0.16          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 6        | 0.16          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 8        | 0.16          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 12       | 0.16          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 13       | 0.16          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 14       | 0.16          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 16       | 0.16          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 18       | 0.16          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 20       | 0.16          |
| (1,3559) | 1:111:A:VAL:HG21 | 1:115:A:VAL:H  | 6        | 0.16          |
| (1,3559) | 1:111:A:VAL:HG22 | 1:115:A:VAL:H  | 6        | 0.16          |
| (1,3559) | 1:111:A:VAL:HG23 | 1:115:A:VAL:H  | 6        | 0.16          |
| (1,3559) | 1:111:A:VAL:HG21 | 1:115:A:VAL:H  | 8        | 0.16          |
| (1,3559) | 1:111:A:VAL:HG22 | 1:115:A:VAL:H  | 8        | 0.16          |
| (1,3559) | 1:111:A:VAL:HG23 | 1:115:A:VAL:H  | 8        | 0.16          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H  | 16       | 0.16          |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H  | 16       | 0.16          |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H  | 16       | 0.16          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H  | 17       | 0.16          |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H  | 17       | 0.16          |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H  | 17       | 0.16          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H   | 1        | 0.16          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H   | 1        | 0.16          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H   | 1        | 0.16          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H   | 13       | 0.16          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H   | 13       | 0.16          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H   | 13       | 0.16          |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H   | 7        | 0.16          |
| (1,3033) | 1:112:A:PHE:HB2  | 1:106:A:GLY:H  | 18       | 0.16          |
| (1,3033) | 1:112:A:PHE:HB3  | 1:106:A:GLY:H  | 18       | 0.16          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H   | 7        | 0.16          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H   | 7        | 0.16          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H   | 18       | 0.16          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H   | 18       | 0.16          |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H   | 9        | 0.16          |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H   | 9        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11  | 11       | 0.16          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12  | 11       | 0.16          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13  | 11       | 0.16          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11  | 14       | 0.16          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12  | 14       | 0.16          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13  | 14       | 0.16          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2   | 1        | 0.16          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3   | 1        | 0.16          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2   | 1        | 0.16          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3   | 1        | 0.16          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2   | 2        | 0.16          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3   | 2        | 0.16          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2   | 2        | 0.16          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3   | 2        | 0.16          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2   | 18       | 0.16          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3   | 18       | 0.16          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2   | 18       | 0.16          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3   | 18       | 0.16          |
| (1,2746) | 1:119:A:VAL:HG21 | 1:15:A:SER:HA    | 12       | 0.16          |
| (1,2746) | 1:119:A:VAL:HG22 | 1:15:A:SER:HA    | 12       | 0.16          |
| (1,2746) | 1:119:A:VAL:HG23 | 1:15:A:SER:HA    | 12       | 0.16          |
| (1,2653) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HB   | 6        | 0.16          |
| (1,2653) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HB   | 6        | 0.16          |
| (1,2653) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HB   | 6        | 0.16          |
| (1,2649) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HA   | 3        | 0.16          |
| (1,2649) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HA   | 3        | 0.16          |
| (1,2649) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HA   | 3        | 0.16          |
| (1,2408) | 1:116:A:ARG:HA   | 1:119:A:VAL:HB   | 1        | 0.16          |
| (1,2405) | 1:119:A:VAL:H    | 1:119:A:VAL:HB   | 1        | 0.16          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 6        | 0.16          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 6        | 0.16          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG21 | 17       | 0.16          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG22 | 17       | 0.16          |
| (1,2326) | 1:119:A:VAL:HG21 | 1:115:A:VAL:HG23 | 17       | 0.16          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG21 | 17       | 0.16          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG22 | 17       | 0.16          |
| (1,2326) | 1:119:A:VAL:HG22 | 1:115:A:VAL:HG23 | 17       | 0.16          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG21 | 17       | 0.16          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG22 | 17       | 0.16          |
| (1,2326) | 1:119:A:VAL:HG23 | 1:115:A:VAL:HG23 | 17       | 0.16          |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG21 | 6        | 0.16          |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG22 | 6        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG23 | 6        | 0.16          |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG21 | 8        | 0.16          |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG22 | 8        | 0.16          |
| (1,2257) | 1:115:A:VAL:H    | 1:111:A:VAL:HG23 | 8        | 0.16          |
| (1,2176) | 1:109:A:LEU:HD21 | 1:108:A:SER:HA   | 13       | 0.16          |
| (1,2176) | 1:109:A:LEU:HD22 | 1:108:A:SER:HA   | 13       | 0.16          |
| (1,2176) | 1:109:A:LEU:HD23 | 1:108:A:SER:HA   | 13       | 0.16          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA   | 7        | 0.16          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA   | 7        | 0.16          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA   | 7        | 0.16          |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB2  | 1        | 0.16          |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB3  | 1        | 0.16          |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB2  | 1        | 0.16          |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB3  | 1        | 0.16          |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB2  | 1        | 0.16          |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB3  | 1        | 0.16          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD11  | 10       | 0.16          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD12  | 10       | 0.16          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD13  | 10       | 0.16          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD11  | 10       | 0.16          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD12  | 10       | 0.16          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD13  | 10       | 0.16          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD11  | 10       | 0.16          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD12  | 10       | 0.16          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD13  | 10       | 0.16          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21  | 10       | 0.16          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22  | 10       | 0.16          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23  | 10       | 0.16          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21  | 17       | 0.16          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22  | 17       | 0.16          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23  | 17       | 0.16          |
| (1,991)  | 1:57:A:ILE:H     | 1:42:A:VAL:HB    | 12       | 0.16          |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA2   | 3        | 0.16          |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA3   | 3        | 0.16          |
| (1,877)  | 1:5:A:MET:HG3    | 1:36:A:GLY:HA2   | 3        | 0.16          |
| (1,877)  | 1:5:A:MET:HG3    | 1:36:A:GLY:HA3   | 3        | 0.16          |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA2   | 6        | 0.16          |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA3   | 6        | 0.16          |
| (1,877)  | 1:5:A:MET:HG3    | 1:36:A:GLY:HA2   | 6        | 0.16          |
| (1,877)  | 1:5:A:MET:HG3    | 1:36:A:GLY:HA3   | 6        | 0.16          |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA2   | 10       | 0.16          |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA3   | 10       | 0.16          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA2  | 10       | 0.16          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA3  | 10       | 0.16          |
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA2  | 20       | 0.16          |
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA3  | 20       | 0.16          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA2  | 20       | 0.16          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA3  | 20       | 0.16          |
| (1,821) | 1:33:A:THR:H   | 1:32:A:VAL:HG21 | 17       | 0.16          |
| (1,821) | 1:33:A:THR:H   | 1:32:A:VAL:HG22 | 17       | 0.16          |
| (1,821) | 1:33:A:THR:H   | 1:32:A:VAL:HG23 | 17       | 0.16          |
| (1,810) | 1:33:A:THR:H   | 1:32:A:VAL:HG11 | 11       | 0.16          |
| (1,810) | 1:33:A:THR:H   | 1:32:A:VAL:HG12 | 11       | 0.16          |
| (1,810) | 1:33:A:THR:H   | 1:32:A:VAL:HG13 | 11       | 0.16          |
| (1,793) | 1:31:A:ALA:HB1 | 1:32:A:VAL:HB   | 1        | 0.16          |
| (1,793) | 1:31:A:ALA:HB2 | 1:32:A:VAL:HB   | 1        | 0.16          |
| (1,793) | 1:31:A:ALA:HB3 | 1:32:A:VAL:HB   | 1        | 0.16          |
| (1,793) | 1:31:A:ALA:HB1 | 1:32:A:VAL:HB   | 4        | 0.16          |
| (1,793) | 1:31:A:ALA:HB2 | 1:32:A:VAL:HB   | 4        | 0.16          |
| (1,793) | 1:31:A:ALA:HB3 | 1:32:A:VAL:HB   | 4        | 0.16          |
| (1,793) | 1:31:A:ALA:HB1 | 1:32:A:VAL:HB   | 8        | 0.16          |
| (1,793) | 1:31:A:ALA:HB2 | 1:32:A:VAL:HB   | 8        | 0.16          |
| (1,793) | 1:31:A:ALA:HB3 | 1:32:A:VAL:HB   | 8        | 0.16          |
| (1,793) | 1:31:A:ALA:HB1 | 1:32:A:VAL:HB   | 12       | 0.16          |
| (1,793) | 1:31:A:ALA:HB2 | 1:32:A:VAL:HB   | 12       | 0.16          |
| (1,793) | 1:31:A:ALA:HB3 | 1:32:A:VAL:HB   | 12       | 0.16          |
| (1,793) | 1:31:A:ALA:HB1 | 1:32:A:VAL:HB   | 15       | 0.16          |
| (1,793) | 1:31:A:ALA:HB2 | 1:32:A:VAL:HB   | 15       | 0.16          |
| (1,793) | 1:31:A:ALA:HB3 | 1:32:A:VAL:HB   | 15       | 0.16          |
| (1,793) | 1:31:A:ALA:HB1 | 1:32:A:VAL:HB   | 18       | 0.16          |
| (1,793) | 1:31:A:ALA:HB2 | 1:32:A:VAL:HB   | 18       | 0.16          |
| (1,793) | 1:31:A:ALA:HB3 | 1:32:A:VAL:HB   | 18       | 0.16          |
| (1,793) | 1:31:A:ALA:HB1 | 1:32:A:VAL:HB   | 19       | 0.16          |
| (1,793) | 1:31:A:ALA:HB2 | 1:32:A:VAL:HB   | 19       | 0.16          |
| (1,793) | 1:31:A:ALA:HB3 | 1:32:A:VAL:HB   | 19       | 0.16          |
| (1,744) | 1:1:A:MET:HB2  | 1:30:A:ILE:HB   | 3        | 0.16          |
| (1,744) | 1:1:A:MET:HB3  | 1:30:A:ILE:HB   | 3        | 0.16          |
| (1,634) | 1:24:A:THR:H   | 1:24:A:THR:HB   | 11       | 0.16          |
| (1,633) | 1:62:A:SER:HA  | 1:61:A:THR:HB   | 5        | 0.16          |
| (1,448) | 1:19:A:GLU:H   | 1:16:A:GLN:HB2  | 19       | 0.16          |
| (1,448) | 1:19:A:GLU:H   | 1:16:A:GLN:HB3  | 19       | 0.16          |
| (1,443) | 1:10:A:ARG:HB2 | 1:16:A:GLN:HB2  | 8        | 0.16          |
| (1,443) | 1:10:A:ARG:HB2 | 1:16:A:GLN:HB3  | 8        | 0.16          |
| (1,443) | 1:10:A:ARG:HB3 | 1:16:A:GLN:HB2  | 8        | 0.16          |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3 | 8        | 0.16          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2 | 9        | 0.16          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3 | 9        | 0.16          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2 | 9        | 0.16          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3 | 9        | 0.16          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2 | 13       | 0.16          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3 | 13       | 0.16          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2 | 13       | 0.16          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3 | 13       | 0.16          |
| (1,433)  | 1:50:A:MET:HE1   | 1:16:A:GLN:HA  | 5        | 0.16          |
| (1,433)  | 1:50:A:MET:HE2   | 1:16:A:GLN:HA  | 5        | 0.16          |
| (1,433)  | 1:50:A:MET:HE3   | 1:16:A:GLN:HA  | 5        | 0.16          |
| (1,318)  | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG21 | 10       | 0.16          |
| (1,318)  | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG22 | 10       | 0.16          |
| (1,318)  | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG23 | 10       | 0.16          |
| (1,318)  | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG21 | 10       | 0.16          |
| (1,318)  | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG22 | 10       | 0.16          |
| (1,318)  | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG23 | 10       | 0.16          |
| (1,318)  | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG21 | 10       | 0.16          |
| (1,318)  | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG22 | 10       | 0.16          |
| (1,318)  | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG23 | 10       | 0.16          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1  | 8        | 0.16          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2  | 8        | 0.16          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1  | 13       | 0.16          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2  | 13       | 0.16          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1  | 15       | 0.16          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2  | 15       | 0.16          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1  | 17       | 0.16          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2  | 17       | 0.16          |
| (1,108)  | 1:90:A:TRP:H     | 1:90:A:TRP:HD1 | 20       | 0.16          |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1 | 12       | 0.15          |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1 | 13       | 0.15          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 2        | 0.15          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 5        | 0.15          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 7        | 0.15          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 11       | 0.15          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 17       | 0.15          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H  | 4        | 0.15          |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H  | 4        | 0.15          |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H  | 4        | 0.15          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H  | 5        | 0.15          |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H  | 5        | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H   | 5        | 0.15          |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H    | 3        | 0.15          |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H    | 3        | 0.15          |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H    | 20       | 0.15          |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H    | 20       | 0.15          |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H    | 3        | 0.15          |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H    | 18       | 0.15          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H    | 2        | 0.15          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H    | 2        | 0.15          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H    | 10       | 0.15          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H    | 10       | 0.15          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H    | 12       | 0.15          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H    | 12       | 0.15          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H    | 17       | 0.15          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H    | 17       | 0.15          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H    | 19       | 0.15          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H    | 19       | 0.15          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H    | 20       | 0.15          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H    | 20       | 0.15          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H    | 4        | 0.15          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H    | 4        | 0.15          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H    | 20       | 0.15          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H    | 20       | 0.15          |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H    | 19       | 0.15          |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H    | 19       | 0.15          |
| (1,2836) | 1:4:A:VAL:HB     | 1:4:A:VAL:H     | 6        | 0.15          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11 | 1        | 0.15          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12 | 1        | 0.15          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13 | 1        | 0.15          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11 | 5        | 0.15          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12 | 5        | 0.15          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13 | 5        | 0.15          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2  | 14       | 0.15          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3  | 14       | 0.15          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2  | 14       | 0.15          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3  | 14       | 0.15          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2  | 19       | 0.15          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3  | 19       | 0.15          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2  | 19       | 0.15          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3  | 19       | 0.15          |
| (1,2649) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HA  | 19       | 0.15          |
| (1,2649) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HA  | 19       | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2649) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HA  | 19       | 0.15          |
| (1,2408) | 1:116:A:ARG:HA   | 1:119:A:VAL:HB  | 20       | 0.15          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA  | 11       | 0.15          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA  | 11       | 0.15          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA  | 9        | 0.15          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA  | 9        | 0.15          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA  | 9        | 0.15          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA  | 12       | 0.15          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA  | 12       | 0.15          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA  | 12       | 0.15          |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB2 | 10       | 0.15          |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB3 | 10       | 0.15          |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB2 | 10       | 0.15          |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB3 | 10       | 0.15          |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB2 | 10       | 0.15          |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB3 | 10       | 0.15          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG21 | 10       | 0.15          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG22 | 10       | 0.15          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG23 | 10       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG11 | 11       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG12 | 11       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG13 | 11       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG11 | 11       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG12 | 11       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG13 | 11       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG11 | 11       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG12 | 11       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG13 | 11       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG11 | 16       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG12 | 16       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG21  | 1:76:A:VAL:HG13 | 16       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG11 | 16       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG12 | 16       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG22  | 1:76:A:VAL:HG13 | 16       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG11 | 16       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG12 | 16       | 0.15          |
| (1,1631) | 1:91:A:VAL:HG23  | 1:76:A:VAL:HG13 | 16       | 0.15          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD11 | 20       | 0.15          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD12 | 20       | 0.15          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD13 | 20       | 0.15          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD11 | 20       | 0.15          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD12 | 20       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1476) | 1:7:A:VAL:HG22  | 1:65:A:ILE:HD13 | 20       | 0.15          |
| (1,1476) | 1:7:A:VAL:HG23  | 1:65:A:ILE:HD11 | 20       | 0.15          |
| (1,1476) | 1:7:A:VAL:HG23  | 1:65:A:ILE:HD12 | 20       | 0.15          |
| (1,1476) | 1:7:A:VAL:HG23  | 1:65:A:ILE:HD13 | 20       | 0.15          |
| (1,1355) | 1:47:A:ILE:HG21 | 1:58:A:SER:HA   | 17       | 0.15          |
| (1,1355) | 1:47:A:ILE:HG22 | 1:58:A:SER:HA   | 17       | 0.15          |
| (1,1355) | 1:47:A:ILE:HG23 | 1:58:A:SER:HA   | 17       | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG21 | 4        | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG22 | 4        | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG23 | 4        | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG21 | 6        | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG22 | 6        | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG23 | 6        | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG21 | 8        | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG22 | 8        | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG23 | 8        | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG21 | 18       | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG22 | 18       | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG23 | 18       | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG21 | 19       | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG22 | 19       | 0.15          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG23 | 19       | 0.15          |
| (1,1166) | 1:60:A:GLN:HE21 | 1:50:A:MET:HB2  | 11       | 0.15          |
| (1,1166) | 1:60:A:GLN:HE21 | 1:50:A:MET:HB3  | 11       | 0.15          |
| (1,1166) | 1:60:A:GLN:HE22 | 1:50:A:MET:HB2  | 11       | 0.15          |
| (1,1166) | 1:60:A:GLN:HE22 | 1:50:A:MET:HB3  | 11       | 0.15          |
| (1,991)  | 1:57:A:ILE:H    | 1:42:A:VAL:HB   | 6        | 0.15          |
| (1,991)  | 1:57:A:ILE:H    | 1:42:A:VAL:HB   | 7        | 0.15          |
| (1,991)  | 1:57:A:ILE:H    | 1:42:A:VAL:HB   | 10       | 0.15          |
| (1,991)  | 1:57:A:ILE:H    | 1:42:A:VAL:HB   | 16       | 0.15          |
| (1,928)  | 1:40:A:SER:HA   | 1:38:A:GLU:HA   | 3        | 0.15          |
| (1,928)  | 1:40:A:SER:HA   | 1:38:A:GLU:HA   | 13       | 0.15          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA2  | 17       | 0.15          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA3  | 17       | 0.15          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA2  | 17       | 0.15          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA3  | 17       | 0.15          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG21 | 20       | 0.15          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG22 | 20       | 0.15          |
| (1,821)  | 1:33:A:THR:H    | 1:32:A:VAL:HG23 | 20       | 0.15          |
| (1,793)  | 1:31:A:ALA:HB1  | 1:32:A:VAL:HB   | 11       | 0.15          |
| (1,793)  | 1:31:A:ALA:HB2  | 1:32:A:VAL:HB   | 11       | 0.15          |
| (1,793)  | 1:31:A:ALA:HB3  | 1:32:A:VAL:HB   | 11       | 0.15          |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,793) | 1:31:A:ALA:HB1   | 1:32:A:VAL:HB  | 13       | 0.15          |
| (1,793) | 1:31:A:ALA:HB2   | 1:32:A:VAL:HB  | 13       | 0.15          |
| (1,793) | 1:31:A:ALA:HB3   | 1:32:A:VAL:HB  | 13       | 0.15          |
| (1,649) | 1:24:A:THR:HG21  | 1:25:A:LEU:HA  | 20       | 0.15          |
| (1,649) | 1:24:A:THR:HG22  | 1:25:A:LEU:HA  | 20       | 0.15          |
| (1,649) | 1:24:A:THR:HG23  | 1:25:A:LEU:HA  | 20       | 0.15          |
| (1,634) | 1:24:A:THR:H     | 1:24:A:THR:HB  | 4        | 0.15          |
| (1,634) | 1:24:A:THR:H     | 1:24:A:THR:HB  | 5        | 0.15          |
| (1,633) | 1:62:A:SER:HA    | 1:61:A:THR:HB  | 1        | 0.15          |
| (1,633) | 1:62:A:SER:HA    | 1:61:A:THR:HB  | 12       | 0.15          |
| (1,633) | 1:62:A:SER:HA    | 1:61:A:THR:HB  | 15       | 0.15          |
| (1,633) | 1:62:A:SER:HA    | 1:61:A:THR:HB  | 19       | 0.15          |
| (1,486) | 1:123:A:VAL:HA   | 1:18:A:ALA:HA  | 11       | 0.15          |
| (1,486) | 1:123:A:VAL:HA   | 1:18:A:ALA:HA  | 14       | 0.15          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB2 | 13       | 0.15          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB3 | 13       | 0.15          |
| (1,405) | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB | 1        | 0.15          |
| (1,405) | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB | 1        | 0.15          |
| (1,405) | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB | 1        | 0.15          |
| (1,405) | 1:126:A:LEU:HD11 | 1:130:A:ILE:HB | 3        | 0.15          |
| (1,405) | 1:126:A:LEU:HD12 | 1:130:A:ILE:HB | 3        | 0.15          |
| (1,405) | 1:126:A:LEU:HD13 | 1:130:A:ILE:HB | 3        | 0.15          |
| (1,340) | 1:104:A:PRO:HD2  | 1:8:A:SER:HB2  | 13       | 0.15          |
| (1,340) | 1:104:A:PRO:HD2  | 1:8:A:SER:HB3  | 13       | 0.15          |
| (1,340) | 1:104:A:PRO:HD3  | 1:8:A:SER:HB2  | 13       | 0.15          |
| (1,340) | 1:104:A:PRO:HD3  | 1:8:A:SER:HB3  | 13       | 0.15          |
| (1,318) | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG21 | 20       | 0.15          |
| (1,318) | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG22 | 20       | 0.15          |
| (1,318) | 1:65:A:ILE:HD11  | 1:7:A:VAL:HG23 | 20       | 0.15          |
| (1,318) | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG21 | 20       | 0.15          |
| (1,318) | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG22 | 20       | 0.15          |
| (1,318) | 1:65:A:ILE:HD12  | 1:7:A:VAL:HG23 | 20       | 0.15          |
| (1,318) | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG21 | 20       | 0.15          |
| (1,318) | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG22 | 20       | 0.15          |
| (1,318) | 1:65:A:ILE:HD13  | 1:7:A:VAL:HG23 | 20       | 0.15          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG21 | 16       | 0.15          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG22 | 16       | 0.15          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG23 | 16       | 0.15          |
| (1,249) | 1:4:A:VAL:H      | 1:4:A:VAL:HB   | 6        | 0.15          |
| (1,139) | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1  | 10       | 0.15          |
| (1,139) | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2  | 10       | 0.15          |
| (1,51)  | 1:23:A:LYS:HB2   | 1:25:A:LEU:H   | 5        | 0.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,51)   | 1:23:A:LYS:HB3   | 1:25:A:LEU:H    | 5        | 0.15          |
| (1,51)   | 1:23:A:LYS:HB2   | 1:25:A:LEU:H    | 11       | 0.15          |
| (1,51)   | 1:23:A:LYS:HB3   | 1:25:A:LEU:H    | 11       | 0.15          |
| (1,3676) | 1:126:A:LEU:HD21 | 1:129:A:LYS:H   | 7        | 0.14          |
| (1,3676) | 1:126:A:LEU:HD22 | 1:129:A:LYS:H   | 7        | 0.14          |
| (1,3676) | 1:126:A:LEU:HD23 | 1:129:A:LYS:H   | 7        | 0.14          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H   | 3        | 0.14          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H   | 9        | 0.14          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H   | 19       | 0.14          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H   | 14       | 0.14          |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H   | 14       | 0.14          |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H   | 14       | 0.14          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H   | 18       | 0.14          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H   | 18       | 0.14          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H    | 15       | 0.14          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H    | 15       | 0.14          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H    | 15       | 0.14          |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H    | 1        | 0.14          |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H    | 1        | 0.14          |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H    | 4        | 0.14          |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H    | 12       | 0.14          |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H    | 14       | 0.14          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H    | 14       | 0.14          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H    | 14       | 0.14          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H    | 15       | 0.14          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H    | 15       | 0.14          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H    | 1        | 0.14          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H    | 1        | 0.14          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H    | 14       | 0.14          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H    | 14       | 0.14          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H    | 15       | 0.14          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H    | 15       | 0.14          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H    | 17       | 0.14          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H    | 17       | 0.14          |
| (1,2939) | 1:60:A:GLN:HE21  | 1:22:A:ALA:H    | 16       | 0.14          |
| (1,2939) | 1:60:A:GLN:HE22  | 1:22:A:ALA:H    | 16       | 0.14          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11 | 12       | 0.14          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12 | 12       | 0.14          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13 | 12       | 0.14          |
| (1,2649) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HA  | 6        | 0.14          |
| (1,2649) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HA  | 6        | 0.14          |
| (1,2649) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HA  | 6        | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA  | 16       | 0.14          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA  | 16       | 0.14          |
| (1,2176) | 1:109:A:LEU:HD21 | 1:108:A:SER:HA  | 4        | 0.14          |
| (1,2176) | 1:109:A:LEU:HD22 | 1:108:A:SER:HA  | 4        | 0.14          |
| (1,2176) | 1:109:A:LEU:HD23 | 1:108:A:SER:HA  | 4        | 0.14          |
| (1,2176) | 1:109:A:LEU:HD21 | 1:108:A:SER:HA  | 12       | 0.14          |
| (1,2176) | 1:109:A:LEU:HD22 | 1:108:A:SER:HA  | 12       | 0.14          |
| (1,2176) | 1:109:A:LEU:HD23 | 1:108:A:SER:HA  | 12       | 0.14          |
| (1,2124) | 1:4:A:VAL:HG21   | 1:126:A:LEU:HG  | 14       | 0.14          |
| (1,2124) | 1:4:A:VAL:HG22   | 1:126:A:LEU:HG  | 14       | 0.14          |
| (1,2124) | 1:4:A:VAL:HG23   | 1:126:A:LEU:HG  | 14       | 0.14          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA  | 16       | 0.14          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA  | 16       | 0.14          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA  | 16       | 0.14          |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB2 | 20       | 0.14          |
| (1,2072) | 1:111:A:VAL:HG21 | 1:102:A:GLU:HB3 | 20       | 0.14          |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB2 | 20       | 0.14          |
| (1,2072) | 1:111:A:VAL:HG22 | 1:102:A:GLU:HB3 | 20       | 0.14          |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB2 | 20       | 0.14          |
| (1,2072) | 1:111:A:VAL:HG23 | 1:102:A:GLU:HB3 | 20       | 0.14          |
| (1,2022) | 1:100:A:GLN:H    | 1:98:A:ASP:HA   | 9        | 0.14          |
| (1,1800) | 1:90:A:TRP:HB2   | 1:86:A:LEU:HD11 | 17       | 0.14          |
| (1,1800) | 1:90:A:TRP:HB2   | 1:86:A:LEU:HD12 | 17       | 0.14          |
| (1,1800) | 1:90:A:TRP:HB2   | 1:86:A:LEU:HD13 | 17       | 0.14          |
| (1,1800) | 1:90:A:TRP:HB3   | 1:86:A:LEU:HD11 | 17       | 0.14          |
| (1,1800) | 1:90:A:TRP:HB3   | 1:86:A:LEU:HD12 | 17       | 0.14          |
| (1,1800) | 1:90:A:TRP:HB3   | 1:86:A:LEU:HD13 | 17       | 0.14          |
| (1,1755) | 1:91:A:VAL:HG21  | 1:83:A:GLY:HA2  | 10       | 0.14          |
| (1,1755) | 1:91:A:VAL:HG21  | 1:83:A:GLY:HA3  | 10       | 0.14          |
| (1,1755) | 1:91:A:VAL:HG22  | 1:83:A:GLY:HA2  | 10       | 0.14          |
| (1,1755) | 1:91:A:VAL:HG22  | 1:83:A:GLY:HA3  | 10       | 0.14          |
| (1,1755) | 1:91:A:VAL:HG23  | 1:83:A:GLY:HA2  | 10       | 0.14          |
| (1,1755) | 1:91:A:VAL:HG23  | 1:83:A:GLY:HA3  | 10       | 0.14          |
| (1,1741) | 1:18:A:ALA:H     | 1:79:A:LEU:HD11 | 18       | 0.14          |
| (1,1741) | 1:18:A:ALA:H     | 1:79:A:LEU:HD12 | 18       | 0.14          |
| (1,1741) | 1:18:A:ALA:H     | 1:79:A:LEU:HD13 | 18       | 0.14          |
| (1,1456) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HB   | 13       | 0.14          |
| (1,1456) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HB   | 13       | 0.14          |
| (1,1456) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HB   | 13       | 0.14          |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB2  | 2        | 0.14          |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB3  | 2        | 0.14          |
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB2  | 2        | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB3  | 2        | 0.14          |
| (1,1355) | 1:47:A:ILE:HG21  | 1:58:A:SER:HA   | 5        | 0.14          |
| (1,1355) | 1:47:A:ILE:HG22  | 1:58:A:SER:HA   | 5        | 0.14          |
| (1,1355) | 1:47:A:ILE:HG23  | 1:58:A:SER:HA   | 5        | 0.14          |
| (1,1355) | 1:47:A:ILE:HG21  | 1:58:A:SER:HA   | 8        | 0.14          |
| (1,1355) | 1:47:A:ILE:HG22  | 1:58:A:SER:HA   | 8        | 0.14          |
| (1,1355) | 1:47:A:ILE:HG23  | 1:58:A:SER:HA   | 8        | 0.14          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21 | 12       | 0.14          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22 | 12       | 0.14          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23 | 12       | 0.14          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG21 | 15       | 0.14          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG22 | 15       | 0.14          |
| (1,1304) | 1:19:A:GLU:H     | 1:55:A:ILE:HG23 | 15       | 0.14          |
| (1,991)  | 1:57:A:ILE:H     | 1:42:A:VAL:HB   | 3        | 0.14          |
| (1,991)  | 1:57:A:ILE:H     | 1:42:A:VAL:HB   | 19       | 0.14          |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA2  | 14       | 0.14          |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA3  | 14       | 0.14          |
| (1,877)  | 1:5:A:MET:HG3    | 1:36:A:GLY:HA2  | 14       | 0.14          |
| (1,877)  | 1:5:A:MET:HG3    | 1:36:A:GLY:HA3  | 14       | 0.14          |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA2  | 16       | 0.14          |
| (1,877)  | 1:5:A:MET:HG2    | 1:36:A:GLY:HA3  | 16       | 0.14          |
| (1,877)  | 1:5:A:MET:HG3    | 1:36:A:GLY:HA2  | 16       | 0.14          |
| (1,877)  | 1:5:A:MET:HG3    | 1:36:A:GLY:HA3  | 16       | 0.14          |
| (1,826)  | 1:5:A:MET:HA     | 1:33:A:THR:HA   | 5        | 0.14          |
| (1,649)  | 1:24:A:THR:HG21  | 1:25:A:LEU:HA   | 11       | 0.14          |
| (1,649)  | 1:24:A:THR:HG22  | 1:25:A:LEU:HA   | 11       | 0.14          |
| (1,649)  | 1:24:A:THR:HG23  | 1:25:A:LEU:HA   | 11       | 0.14          |
| (1,634)  | 1:24:A:THR:H     | 1:24:A:THR:HB   | 14       | 0.14          |
| (1,634)  | 1:24:A:THR:H     | 1:24:A:THR:HB   | 17       | 0.14          |
| (1,634)  | 1:24:A:THR:H     | 1:24:A:THR:HB   | 19       | 0.14          |
| (1,633)  | 1:62:A:SER:HA    | 1:61:A:THR:HB   | 7        | 0.14          |
| (1,633)  | 1:62:A:SER:HA    | 1:61:A:THR:HB   | 13       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB1  | 11       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB2  | 11       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB3  | 11       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB1  | 11       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB2  | 11       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB3  | 11       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB1  | 11       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB2  | 11       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB3  | 11       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB1  | 15       | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB2  | 15       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG11 | 1:22:A:ALA:HB3  | 15       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB1  | 15       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB2  | 15       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG12 | 1:22:A:ALA:HB3  | 15       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB1  | 15       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB2  | 15       | 0.14          |
| (1,569)  | 1:123:A:VAL:HG13 | 1:22:A:ALA:HB3  | 15       | 0.14          |
| (1,448)  | 1:19:A:GLU:H     | 1:16:A:GLN:HB2  | 12       | 0.14          |
| (1,448)  | 1:19:A:GLU:H     | 1:16:A:GLN:HB3  | 12       | 0.14          |
| (1,448)  | 1:19:A:GLU:H     | 1:16:A:GLN:HB2  | 20       | 0.14          |
| (1,448)  | 1:19:A:GLU:H     | 1:16:A:GLN:HB3  | 20       | 0.14          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2  | 4        | 0.14          |
| (1,443)  | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3  | 4        | 0.14          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2  | 4        | 0.14          |
| (1,443)  | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3  | 4        | 0.14          |
| (1,433)  | 1:50:A:MET:HE1   | 1:16:A:GLN:HA   | 16       | 0.14          |
| (1,433)  | 1:50:A:MET:HE2   | 1:16:A:GLN:HA   | 16       | 0.14          |
| (1,433)  | 1:50:A:MET:HE3   | 1:16:A:GLN:HA   | 16       | 0.14          |
| (1,433)  | 1:50:A:MET:HE1   | 1:16:A:GLN:HA   | 17       | 0.14          |
| (1,433)  | 1:50:A:MET:HE2   | 1:16:A:GLN:HA   | 17       | 0.14          |
| (1,433)  | 1:50:A:MET:HE3   | 1:16:A:GLN:HA   | 17       | 0.14          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE1  | 5        | 0.14          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE2  | 5        | 0.14          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1   | 9        | 0.14          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2   | 9        | 0.14          |
| (1,108)  | 1:90:A:TRP:H     | 1:90:A:TRP:HD1  | 12       | 0.14          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD11 | 7        | 0.14          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD12 | 7        | 0.14          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD13 | 7        | 0.14          |
| (1,37)   | 1:90:A:TRP:HB2   | 1:86:A:LEU:HD11 | 17       | 0.14          |
| (1,37)   | 1:90:A:TRP:HB2   | 1:86:A:LEU:HD12 | 17       | 0.14          |
| (1,37)   | 1:90:A:TRP:HB2   | 1:86:A:LEU:HD13 | 17       | 0.14          |
| (1,37)   | 1:90:A:TRP:HB3   | 1:86:A:LEU:HD11 | 17       | 0.14          |
| (1,37)   | 1:90:A:TRP:HB3   | 1:86:A:LEU:HD12 | 17       | 0.14          |
| (1,37)   | 1:90:A:TRP:HB3   | 1:86:A:LEU:HD13 | 17       | 0.14          |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1  | 5        | 0.13          |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1  | 17       | 0.13          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1  | 9        | 0.13          |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1  | 9        | 0.13          |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1  | 9        | 0.13          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H   | 8        | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H   | 8        | 0.13          |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H   | 8        | 0.13          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H   | 5        | 0.13          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H   | 5        | 0.13          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H   | 6        | 0.13          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H   | 6        | 0.13          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H   | 10       | 0.13          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H   | 10       | 0.13          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H   | 17       | 0.13          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H   | 17       | 0.13          |
| (1,3504) | 1:43:A:HIS:HE1   | 1:105:A:ASP:H   | 12       | 0.13          |
| (1,3399) | 1:91:A:VAL:HG11  | 1:90:A:TRP:H    | 7        | 0.13          |
| (1,3399) | 1:91:A:VAL:HG12  | 1:90:A:TRP:H    | 7        | 0.13          |
| (1,3399) | 1:91:A:VAL:HG13  | 1:90:A:TRP:H    | 7        | 0.13          |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H    | 9        | 0.13          |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H    | 9        | 0.13          |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H    | 19       | 0.13          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H    | 1        | 0.13          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H    | 1        | 0.13          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H    | 4        | 0.13          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H    | 4        | 0.13          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H    | 5        | 0.13          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H    | 5        | 0.13          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H    | 9        | 0.13          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H    | 9        | 0.13          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H    | 18       | 0.13          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H    | 18       | 0.13          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2  | 3        | 0.13          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3  | 3        | 0.13          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2  | 3        | 0.13          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3  | 3        | 0.13          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2  | 5        | 0.13          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3  | 5        | 0.13          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2  | 5        | 0.13          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3  | 5        | 0.13          |
| (1,2779) | 1:79:A:LEU:HB2   | 1:78:A:SER:HB2  | 19       | 0.13          |
| (1,2779) | 1:79:A:LEU:HB2   | 1:78:A:SER:HB3  | 19       | 0.13          |
| (1,2779) | 1:79:A:LEU:HB3   | 1:78:A:SER:HB2  | 19       | 0.13          |
| (1,2779) | 1:79:A:LEU:HB3   | 1:78:A:SER:HB3  | 19       | 0.13          |
| (1,2772) | 1:4:A:VAL:HG21   | 1:77:A:ILE:HG12 | 1        | 0.13          |
| (1,2772) | 1:4:A:VAL:HG21   | 1:77:A:ILE:HG13 | 1        | 0.13          |
| (1,2772) | 1:4:A:VAL:HG22   | 1:77:A:ILE:HG12 | 1        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2772) | 1:4:A:VAL:HG22   | 1:77:A:ILE:HG13  | 1        | 0.13          |
| (1,2772) | 1:4:A:VAL:HG23   | 1:77:A:ILE:HG12  | 1        | 0.13          |
| (1,2772) | 1:4:A:VAL:HG23   | 1:77:A:ILE:HG13  | 1        | 0.13          |
| (1,2745) | 1:79:A:LEU:HG    | 1:15:A:SER:HA    | 18       | 0.13          |
| (1,2653) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HB   | 3        | 0.13          |
| (1,2653) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HB   | 3        | 0.13          |
| (1,2653) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HB   | 3        | 0.13          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 8        | 0.13          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 8        | 0.13          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 8        | 0.13          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 12       | 0.13          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 12       | 0.13          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 12       | 0.13          |
| (1,2408) | 1:116:A:ARG:HA   | 1:119:A:VAL:HB   | 19       | 0.13          |
| (1,2402) | 1:118:A:GLN:HE21 | 1:119:A:VAL:HA   | 9        | 0.13          |
| (1,2402) | 1:118:A:GLN:HE22 | 1:119:A:VAL:HA   | 9        | 0.13          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA   | 15       | 0.13          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA   | 15       | 0.13          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA   | 15       | 0.13          |
| (1,2022) | 1:100:A:GLN:H    | 1:98:A:ASP:HA    | 19       | 0.13          |
| (1,1980) | 1:91:A:VAL:H     | 1:96:A:PHE:HB2   | 3        | 0.13          |
| (1,1980) | 1:91:A:VAL:H     | 1:96:A:PHE:HB3   | 3        | 0.13          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2   | 6        | 0.13          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3   | 6        | 0.13          |
| (1,1741) | 1:18:A:ALA:H     | 1:79:A:LEU:HD11  | 8        | 0.13          |
| (1,1741) | 1:18:A:ALA:H     | 1:79:A:LEU:HD12  | 8        | 0.13          |
| (1,1741) | 1:18:A:ALA:H     | 1:79:A:LEU:HD13  | 8        | 0.13          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG21  | 9        | 0.13          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG22  | 9        | 0.13          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG23  | 9        | 0.13          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG21  | 13       | 0.13          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG22  | 13       | 0.13          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG23  | 13       | 0.13          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD11  | 8        | 0.13          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD12  | 8        | 0.13          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD13  | 8        | 0.13          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD11  | 8        | 0.13          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD12  | 8        | 0.13          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD13  | 8        | 0.13          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD11  | 8        | 0.13          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD12  | 8        | 0.13          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD13  | 8        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1364) | 1:60:A:GLN:HB2  | 1:58:A:SER:HB2  | 6        | 0.13          |
| (1,1364) | 1:60:A:GLN:HB2  | 1:58:A:SER:HB3  | 6        | 0.13          |
| (1,1364) | 1:60:A:GLN:HB3  | 1:58:A:SER:HB2  | 6        | 0.13          |
| (1,1364) | 1:60:A:GLN:HB3  | 1:58:A:SER:HB3  | 6        | 0.13          |
| (1,1355) | 1:47:A:ILE:HG21 | 1:58:A:SER:HA   | 9        | 0.13          |
| (1,1355) | 1:47:A:ILE:HG22 | 1:58:A:SER:HA   | 9        | 0.13          |
| (1,1355) | 1:47:A:ILE:HG23 | 1:58:A:SER:HA   | 9        | 0.13          |
| (1,1355) | 1:47:A:ILE:HG21 | 1:58:A:SER:HA   | 15       | 0.13          |
| (1,1355) | 1:47:A:ILE:HG22 | 1:58:A:SER:HA   | 15       | 0.13          |
| (1,1355) | 1:47:A:ILE:HG23 | 1:58:A:SER:HA   | 15       | 0.13          |
| (1,1355) | 1:47:A:ILE:HG21 | 1:58:A:SER:HA   | 19       | 0.13          |
| (1,1355) | 1:47:A:ILE:HG22 | 1:58:A:SER:HA   | 19       | 0.13          |
| (1,1355) | 1:47:A:ILE:HG23 | 1:58:A:SER:HA   | 19       | 0.13          |
| (1,1340) | 1:41:A:ARG:HG2  | 1:57:A:ILE:HD11 | 11       | 0.13          |
| (1,1340) | 1:41:A:ARG:HG2  | 1:57:A:ILE:HD12 | 11       | 0.13          |
| (1,1340) | 1:41:A:ARG:HG2  | 1:57:A:ILE:HD13 | 11       | 0.13          |
| (1,1340) | 1:41:A:ARG:HG3  | 1:57:A:ILE:HD11 | 11       | 0.13          |
| (1,1340) | 1:41:A:ARG:HG3  | 1:57:A:ILE:HD12 | 11       | 0.13          |
| (1,1340) | 1:41:A:ARG:HG3  | 1:57:A:ILE:HD13 | 11       | 0.13          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG21 | 1        | 0.13          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG22 | 1        | 0.13          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG23 | 1        | 0.13          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG21 | 5        | 0.13          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG22 | 5        | 0.13          |
| (1,1304) | 1:19:A:GLU:H    | 1:55:A:ILE:HG23 | 5        | 0.13          |
| (1,1133) | 1:50:A:MET:HG2  | 1:48:A:ALA:HB1  | 16       | 0.13          |
| (1,1133) | 1:50:A:MET:HG2  | 1:48:A:ALA:HB2  | 16       | 0.13          |
| (1,1133) | 1:50:A:MET:HG2  | 1:48:A:ALA:HB3  | 16       | 0.13          |
| (1,1133) | 1:50:A:MET:HG3  | 1:48:A:ALA:HB1  | 16       | 0.13          |
| (1,1133) | 1:50:A:MET:HG3  | 1:48:A:ALA:HB2  | 16       | 0.13          |
| (1,1133) | 1:50:A:MET:HG3  | 1:48:A:ALA:HB3  | 16       | 0.13          |
| (1,991)  | 1:57:A:ILE:H    | 1:42:A:VAL:HB   | 1        | 0.13          |
| (1,991)  | 1:57:A:ILE:H    | 1:42:A:VAL:HB   | 14       | 0.13          |
| (1,991)  | 1:57:A:ILE:H    | 1:42:A:VAL:HB   | 15       | 0.13          |
| (1,928)  | 1:40:A:SER:HA   | 1:38:A:GLU:HA   | 5        | 0.13          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA2  | 2        | 0.13          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA3  | 2        | 0.13          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA2  | 2        | 0.13          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA3  | 2        | 0.13          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA2  | 4        | 0.13          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA3  | 4        | 0.13          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA2  | 4        | 0.13          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA3  | 4        | 0.13          |
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA2  | 11       | 0.13          |
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA3  | 11       | 0.13          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA2  | 11       | 0.13          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA3  | 11       | 0.13          |
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA2  | 18       | 0.13          |
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA3  | 18       | 0.13          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA2  | 18       | 0.13          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA3  | 18       | 0.13          |
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA2  | 19       | 0.13          |
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA3  | 19       | 0.13          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA2  | 19       | 0.13          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA3  | 19       | 0.13          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG21 | 14       | 0.13          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG22 | 14       | 0.13          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG23 | 14       | 0.13          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG21 | 14       | 0.13          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG22 | 14       | 0.13          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG23 | 14       | 0.13          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG21 | 17       | 0.13          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG22 | 17       | 0.13          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG23 | 17       | 0.13          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG21 | 17       | 0.13          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG22 | 17       | 0.13          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG23 | 17       | 0.13          |
| (1,822) | 1:31:A:ALA:H   | 1:32:A:VAL:HG21 | 5        | 0.13          |
| (1,822) | 1:31:A:ALA:H   | 1:32:A:VAL:HG22 | 5        | 0.13          |
| (1,822) | 1:31:A:ALA:H   | 1:32:A:VAL:HG23 | 5        | 0.13          |
| (1,821) | 1:33:A:THR:H   | 1:32:A:VAL:HG21 | 19       | 0.13          |
| (1,821) | 1:33:A:THR:H   | 1:32:A:VAL:HG22 | 19       | 0.13          |
| (1,821) | 1:33:A:THR:H   | 1:32:A:VAL:HG23 | 19       | 0.13          |
| (1,802) | 1:33:A:THR:HA  | 1:32:A:VAL:HG11 | 17       | 0.13          |
| (1,802) | 1:33:A:THR:HA  | 1:32:A:VAL:HG12 | 17       | 0.13          |
| (1,802) | 1:33:A:THR:HA  | 1:32:A:VAL:HG13 | 17       | 0.13          |
| (1,795) | 1:6:A:PHE:HE1  | 1:32:A:VAL:HB   | 5        | 0.13          |
| (1,795) | 1:6:A:PHE:HE2  | 1:32:A:VAL:HB   | 5        | 0.13          |
| (1,744) | 1:1:A:MET:HB2  | 1:30:A:ILE:HB   | 1        | 0.13          |
| (1,744) | 1:1:A:MET:HB3  | 1:30:A:ILE:HB   | 1        | 0.13          |
| (1,744) | 1:1:A:MET:HB2  | 1:30:A:ILE:HB   | 5        | 0.13          |
| (1,744) | 1:1:A:MET:HB3  | 1:30:A:ILE:HB   | 5        | 0.13          |
| (1,744) | 1:1:A:MET:HB2  | 1:30:A:ILE:HB   | 13       | 0.13          |
| (1,744) | 1:1:A:MET:HB3  | 1:30:A:ILE:HB   | 13       | 0.13          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,649) | 1:24:A:THR:HG21 | 1:25:A:LEU:HA  | 2        | 0.13          |
| (1,649) | 1:24:A:THR:HG22 | 1:25:A:LEU:HA  | 2        | 0.13          |
| (1,649) | 1:24:A:THR:HG23 | 1:25:A:LEU:HA  | 2        | 0.13          |
| (1,649) | 1:24:A:THR:HG21 | 1:25:A:LEU:HA  | 5        | 0.13          |
| (1,649) | 1:24:A:THR:HG22 | 1:25:A:LEU:HA  | 5        | 0.13          |
| (1,649) | 1:24:A:THR:HG23 | 1:25:A:LEU:HA  | 5        | 0.13          |
| (1,649) | 1:24:A:THR:HG21 | 1:25:A:LEU:HA  | 14       | 0.13          |
| (1,649) | 1:24:A:THR:HG22 | 1:25:A:LEU:HA  | 14       | 0.13          |
| (1,649) | 1:24:A:THR:HG23 | 1:25:A:LEU:HA  | 14       | 0.13          |
| (1,649) | 1:24:A:THR:HG21 | 1:25:A:LEU:HA  | 18       | 0.13          |
| (1,649) | 1:24:A:THR:HG22 | 1:25:A:LEU:HA  | 18       | 0.13          |
| (1,649) | 1:24:A:THR:HG23 | 1:25:A:LEU:HA  | 18       | 0.13          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 1        | 0.13          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 6        | 0.13          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 9        | 0.13          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 12       | 0.13          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 20       | 0.13          |
| (1,633) | 1:62:A:SER:HA   | 1:61:A:THR:HB  | 17       | 0.13          |
| (1,633) | 1:62:A:SER:HA   | 1:61:A:THR:HB  | 18       | 0.13          |
| (1,486) | 1:123:A:VAL:HA  | 1:18:A:ALA:HA  | 13       | 0.13          |
| (1,486) | 1:123:A:VAL:HA  | 1:18:A:ALA:HA  | 15       | 0.13          |
| (1,443) | 1:10:A:ARG:HB2  | 1:16:A:GLN:HB2 | 1        | 0.13          |
| (1,443) | 1:10:A:ARG:HB2  | 1:16:A:GLN:HB3 | 1        | 0.13          |
| (1,443) | 1:10:A:ARG:HB3  | 1:16:A:GLN:HB2 | 1        | 0.13          |
| (1,443) | 1:10:A:ARG:HB3  | 1:16:A:GLN:HB3 | 1        | 0.13          |
| (1,318) | 1:65:A:ILE:HD11 | 1:7:A:VAL:HG21 | 8        | 0.13          |
| (1,318) | 1:65:A:ILE:HD11 | 1:7:A:VAL:HG22 | 8        | 0.13          |
| (1,318) | 1:65:A:ILE:HD11 | 1:7:A:VAL:HG23 | 8        | 0.13          |
| (1,318) | 1:65:A:ILE:HD12 | 1:7:A:VAL:HG21 | 8        | 0.13          |
| (1,318) | 1:65:A:ILE:HD12 | 1:7:A:VAL:HG22 | 8        | 0.13          |
| (1,318) | 1:65:A:ILE:HD12 | 1:7:A:VAL:HG23 | 8        | 0.13          |
| (1,318) | 1:65:A:ILE:HD13 | 1:7:A:VAL:HG21 | 8        | 0.13          |
| (1,318) | 1:65:A:ILE:HD13 | 1:7:A:VAL:HG22 | 8        | 0.13          |
| (1,318) | 1:65:A:ILE:HD13 | 1:7:A:VAL:HG23 | 8        | 0.13          |
| (1,267) | 1:76:A:VAL:HA   | 1:4:A:VAL:HG21 | 8        | 0.13          |
| (1,267) | 1:76:A:VAL:HA   | 1:4:A:VAL:HG22 | 8        | 0.13          |
| (1,267) | 1:76:A:VAL:HA   | 1:4:A:VAL:HG23 | 8        | 0.13          |
| (1,263) | 1:77:A:ILE:HG12 | 1:4:A:VAL:HG21 | 1        | 0.13          |
| (1,263) | 1:77:A:ILE:HG12 | 1:4:A:VAL:HG22 | 1        | 0.13          |
| (1,263) | 1:77:A:ILE:HG12 | 1:4:A:VAL:HG23 | 1        | 0.13          |
| (1,263) | 1:77:A:ILE:HG13 | 1:4:A:VAL:HG21 | 1        | 0.13          |
| (1,263) | 1:77:A:ILE:HG13 | 1:4:A:VAL:HG22 | 1        | 0.13          |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (1,263)  | 1:77:A:ILE:HG13  | 1:4:A:VAL:HG23 | 1        | 0.13          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE1 | 15       | 0.13          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE2 | 15       | 0.13          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE1 | 18       | 0.13          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE2 | 18       | 0.13          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE1 | 20       | 0.13          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE2 | 20       | 0.13          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1  | 7        | 0.13          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2  | 7        | 0.13          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2 | 13       | 0.13          |
| (1,44)   | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3 | 13       | 0.13          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2 | 13       | 0.13          |
| (1,44)   | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3 | 13       | 0.13          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2 | 13       | 0.13          |
| (1,44)   | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3 | 13       | 0.13          |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1 | 2        | 0.12          |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1 | 14       | 0.12          |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1 | 19       | 0.12          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1 | 3        | 0.12          |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1 | 3        | 0.12          |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1 | 3        | 0.12          |
| (1,3666) | 1:130:A:ILE:HD11 | 1:128:A:ALA:H  | 7        | 0.12          |
| (1,3666) | 1:130:A:ILE:HD12 | 1:128:A:ALA:H  | 7        | 0.12          |
| (1,3666) | 1:130:A:ILE:HD13 | 1:128:A:ALA:H  | 7        | 0.12          |
| (1,3666) | 1:130:A:ILE:HD11 | 1:128:A:ALA:H  | 17       | 0.12          |
| (1,3666) | 1:130:A:ILE:HD12 | 1:128:A:ALA:H  | 17       | 0.12          |
| (1,3666) | 1:130:A:ILE:HD13 | 1:128:A:ALA:H  | 17       | 0.12          |
| (1,3562) | 1:115:A:VAL:HB   | 1:115:A:VAL:H  | 10       | 0.12          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H  | 2        | 0.12          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H  | 2        | 0.12          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H  | 7        | 0.12          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H  | 7        | 0.12          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H  | 11       | 0.12          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H  | 11       | 0.12          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H  | 13       | 0.12          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H  | 13       | 0.12          |
| (1,3504) | 1:43:A:HIS:HE1   | 1:105:A:ASP:H  | 13       | 0.12          |
| (1,3426) | 1:76:A:VAL:HG21  | 1:94:A:GLU:H   | 13       | 0.12          |
| (1,3426) | 1:76:A:VAL:HG22  | 1:94:A:GLU:H   | 13       | 0.12          |
| (1,3426) | 1:76:A:VAL:HG23  | 1:94:A:GLU:H   | 13       | 0.12          |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H   | 12       | 0.12          |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H   | 12       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H     | 2        | 0.12          |
| (1,3033) | 1:112:A:PHE:HB2  | 1:106:A:GLY:H    | 2        | 0.12          |
| (1,3033) | 1:112:A:PHE:HB3  | 1:106:A:GLY:H    | 2        | 0.12          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H     | 11       | 0.12          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H     | 11       | 0.12          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H     | 7        | 0.12          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H     | 7        | 0.12          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H     | 13       | 0.12          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H     | 13       | 0.12          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H     | 19       | 0.12          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H     | 19       | 0.12          |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H     | 3        | 0.12          |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H     | 3        | 0.12          |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H     | 6        | 0.12          |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H     | 6        | 0.12          |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H     | 15       | 0.12          |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H     | 15       | 0.12          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD11  | 6        | 0.12          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD12  | 6        | 0.12          |
| (1,2781) | 1:35:A:SER:H     | 1:79:A:LEU:HD13  | 6        | 0.12          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2   | 6        | 0.12          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3   | 6        | 0.12          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2   | 6        | 0.12          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3   | 6        | 0.12          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 10       | 0.12          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 10       | 0.12          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 10       | 0.12          |
| (1,2414) | 1:18:A:ALA:HA    | 1:119:A:VAL:HG11 | 19       | 0.12          |
| (1,2414) | 1:18:A:ALA:HA    | 1:119:A:VAL:HG12 | 19       | 0.12          |
| (1,2414) | 1:18:A:ALA:HA    | 1:119:A:VAL:HG13 | 19       | 0.12          |
| (1,2246) | 1:114:A:THR:HG21 | 1:111:A:VAL:HG21 | 9        | 0.12          |
| (1,2246) | 1:114:A:THR:HG21 | 1:111:A:VAL:HG22 | 9        | 0.12          |
| (1,2246) | 1:114:A:THR:HG21 | 1:111:A:VAL:HG23 | 9        | 0.12          |
| (1,2246) | 1:114:A:THR:HG22 | 1:111:A:VAL:HG21 | 9        | 0.12          |
| (1,2246) | 1:114:A:THR:HG22 | 1:111:A:VAL:HG22 | 9        | 0.12          |
| (1,2246) | 1:114:A:THR:HG22 | 1:111:A:VAL:HG23 | 9        | 0.12          |
| (1,2246) | 1:114:A:THR:HG23 | 1:111:A:VAL:HG21 | 9        | 0.12          |
| (1,2246) | 1:114:A:THR:HG23 | 1:111:A:VAL:HG22 | 9        | 0.12          |
| (1,2246) | 1:114:A:THR:HG23 | 1:111:A:VAL:HG23 | 9        | 0.12          |
| (1,2144) | 1:10:A:ARG:HB2   | 1:104:A:PRO:HD2  | 3        | 0.12          |
| (1,2144) | 1:10:A:ARG:HB2   | 1:104:A:PRO:HD3  | 3        | 0.12          |
| (1,2144) | 1:10:A:ARG:HB3   | 1:104:A:PRO:HD2  | 3        | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2144) | 1:10:A:ARG:HB3   | 1:104:A:PRO:HD3 | 3        | 0.12          |
| (1,2103) | 1:8:A:SER:HB2    | 1:103:A:ASP:HB2 | 12       | 0.12          |
| (1,2103) | 1:8:A:SER:HB2    | 1:103:A:ASP:HB3 | 12       | 0.12          |
| (1,2103) | 1:8:A:SER:HB3    | 1:103:A:ASP:HB2 | 12       | 0.12          |
| (1,2103) | 1:8:A:SER:HB3    | 1:103:A:ASP:HB3 | 12       | 0.12          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA  | 11       | 0.12          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA  | 11       | 0.12          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA  | 11       | 0.12          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2  | 2        | 0.12          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3  | 2        | 0.12          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2  | 15       | 0.12          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3  | 15       | 0.12          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2  | 19       | 0.12          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3  | 19       | 0.12          |
| (1,1756) | 1:86:A:LEU:HD11  | 1:84:A:VAL:HA   | 10       | 0.12          |
| (1,1756) | 1:86:A:LEU:HD12  | 1:84:A:VAL:HA   | 10       | 0.12          |
| (1,1756) | 1:86:A:LEU:HD13  | 1:84:A:VAL:HA   | 10       | 0.12          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG21 | 8        | 0.12          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG22 | 8        | 0.12          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG23 | 8        | 0.12          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG21 | 18       | 0.12          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG22 | 18       | 0.12          |
| (1,1701) | 1:101:A:LEU:HG   | 1:77:A:ILE:HG23 | 18       | 0.12          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD11 | 19       | 0.12          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD12 | 19       | 0.12          |
| (1,1476) | 1:7:A:VAL:HG21   | 1:65:A:ILE:HD13 | 19       | 0.12          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD11 | 19       | 0.12          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD12 | 19       | 0.12          |
| (1,1476) | 1:7:A:VAL:HG22   | 1:65:A:ILE:HD13 | 19       | 0.12          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD11 | 19       | 0.12          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD12 | 19       | 0.12          |
| (1,1476) | 1:7:A:VAL:HG23   | 1:65:A:ILE:HD13 | 19       | 0.12          |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB2  | 7        | 0.12          |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB3  | 7        | 0.12          |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB2  | 9        | 0.12          |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB3  | 9        | 0.12          |
| (1,1355) | 1:47:A:ILE:HG21  | 1:58:A:SER:HA   | 1        | 0.12          |
| (1,1355) | 1:47:A:ILE:HG22  | 1:58:A:SER:HA   | 1        | 0.12          |
| (1,1355) | 1:47:A:ILE:HG23  | 1:58:A:SER:HA   | 1        | 0.12          |
| (1,1355) | 1:47:A:ILE:HG21  | 1:58:A:SER:HA   | 3        | 0.12          |
| (1,1355) | 1:47:A:ILE:HG22  | 1:58:A:SER:HA   | 3        | 0.12          |
| (1,1355) | 1:47:A:ILE:HG23  | 1:58:A:SER:HA   | 3        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1355) | 1:47:A:ILE:HG21 | 1:58:A:SER:HA   | 12       | 0.12          |
| (1,1355) | 1:47:A:ILE:HG22 | 1:58:A:SER:HA   | 12       | 0.12          |
| (1,1355) | 1:47:A:ILE:HG23 | 1:58:A:SER:HA   | 12       | 0.12          |
| (1,1355) | 1:47:A:ILE:HG21 | 1:58:A:SER:HA   | 14       | 0.12          |
| (1,1355) | 1:47:A:ILE:HG22 | 1:58:A:SER:HA   | 14       | 0.12          |
| (1,1355) | 1:47:A:ILE:HG23 | 1:58:A:SER:HA   | 14       | 0.12          |
| (1,1355) | 1:47:A:ILE:HG21 | 1:58:A:SER:HA   | 18       | 0.12          |
| (1,1355) | 1:47:A:ILE:HG22 | 1:58:A:SER:HA   | 18       | 0.12          |
| (1,1355) | 1:47:A:ILE:HG23 | 1:58:A:SER:HA   | 18       | 0.12          |
| (1,1253) | 1:24:A:THR:HB   | 1:54:A:GLY:HA2  | 10       | 0.12          |
| (1,1253) | 1:24:A:THR:HB   | 1:54:A:GLY:HA3  | 10       | 0.12          |
| (1,928)  | 1:40:A:SER:HA   | 1:38:A:GLU:HA   | 8        | 0.12          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA2  | 7        | 0.12          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA3  | 7        | 0.12          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA2  | 7        | 0.12          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA3  | 7        | 0.12          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA2  | 8        | 0.12          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA3  | 8        | 0.12          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA2  | 8        | 0.12          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA3  | 8        | 0.12          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA2  | 13       | 0.12          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA3  | 13       | 0.12          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA2  | 13       | 0.12          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA3  | 13       | 0.12          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA2  | 15       | 0.12          |
| (1,877)  | 1:5:A:MET:HG2   | 1:36:A:GLY:HA3  | 15       | 0.12          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA2  | 15       | 0.12          |
| (1,877)  | 1:5:A:MET:HG3   | 1:36:A:GLY:HA3  | 15       | 0.12          |
| (1,826)  | 1:5:A:MET:HA    | 1:33:A:THR:HA   | 14       | 0.12          |
| (1,826)  | 1:5:A:MET:HA    | 1:33:A:THR:HA   | 18       | 0.12          |
| (1,823)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG21 | 4        | 0.12          |
| (1,823)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG22 | 4        | 0.12          |
| (1,823)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG23 | 4        | 0.12          |
| (1,823)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG21 | 4        | 0.12          |
| (1,823)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG22 | 4        | 0.12          |
| (1,823)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG23 | 4        | 0.12          |
| (1,744)  | 1:1:A:MET:HB2   | 1:30:A:ILE:HB   | 6        | 0.12          |
| (1,744)  | 1:1:A:MET:HB3   | 1:30:A:ILE:HB   | 6        | 0.12          |
| (1,744)  | 1:1:A:MET:HB2   | 1:30:A:ILE:HB   | 8        | 0.12          |
| (1,744)  | 1:1:A:MET:HB3   | 1:30:A:ILE:HB   | 8        | 0.12          |
| (1,744)  | 1:1:A:MET:HB2   | 1:30:A:ILE:HB   | 17       | 0.12          |
| (1,744)  | 1:1:A:MET:HB3   | 1:30:A:ILE:HB   | 17       | 0.12          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,649) | 1:24:A:THR:HG21 | 1:25:A:LEU:HA  | 4        | 0.12          |
| (1,649) | 1:24:A:THR:HG22 | 1:25:A:LEU:HA  | 4        | 0.12          |
| (1,649) | 1:24:A:THR:HG23 | 1:25:A:LEU:HA  | 4        | 0.12          |
| (1,649) | 1:24:A:THR:HG21 | 1:25:A:LEU:HA  | 10       | 0.12          |
| (1,649) | 1:24:A:THR:HG22 | 1:25:A:LEU:HA  | 10       | 0.12          |
| (1,649) | 1:24:A:THR:HG23 | 1:25:A:LEU:HA  | 10       | 0.12          |
| (1,649) | 1:24:A:THR:HG21 | 1:25:A:LEU:HA  | 17       | 0.12          |
| (1,649) | 1:24:A:THR:HG22 | 1:25:A:LEU:HA  | 17       | 0.12          |
| (1,649) | 1:24:A:THR:HG23 | 1:25:A:LEU:HA  | 17       | 0.12          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 2        | 0.12          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 3        | 0.12          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 7        | 0.12          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 8        | 0.12          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 13       | 0.12          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 15       | 0.12          |
| (1,634) | 1:24:A:THR:H    | 1:24:A:THR:HB  | 16       | 0.12          |
| (1,633) | 1:62:A:SER:HA   | 1:61:A:THR:HB  | 6        | 0.12          |
| (1,631) | 1:27:A:ALA:HB1  | 1:24:A:THR:HB  | 13       | 0.12          |
| (1,631) | 1:27:A:ALA:HB2  | 1:24:A:THR:HB  | 13       | 0.12          |
| (1,631) | 1:27:A:ALA:HB3  | 1:24:A:THR:HB  | 13       | 0.12          |
| (1,448) | 1:19:A:GLU:H    | 1:16:A:GLN:HB2 | 8        | 0.12          |
| (1,448) | 1:19:A:GLU:H    | 1:16:A:GLN:HB3 | 8        | 0.12          |
| (1,446) | 1:62:A:SER:HA   | 1:16:A:GLN:HB2 | 4        | 0.12          |
| (1,446) | 1:62:A:SER:HA   | 1:16:A:GLN:HB3 | 4        | 0.12          |
| (1,433) | 1:50:A:MET:HE1  | 1:16:A:GLN:HA  | 1        | 0.12          |
| (1,433) | 1:50:A:MET:HE2  | 1:16:A:GLN:HA  | 1        | 0.12          |
| (1,433) | 1:50:A:MET:HE3  | 1:16:A:GLN:HA  | 1        | 0.12          |
| (1,433) | 1:50:A:MET:HE1  | 1:16:A:GLN:HA  | 2        | 0.12          |
| (1,433) | 1:50:A:MET:HE2  | 1:16:A:GLN:HA  | 2        | 0.12          |
| (1,433) | 1:50:A:MET:HE3  | 1:16:A:GLN:HA  | 2        | 0.12          |
| (1,433) | 1:50:A:MET:HE1  | 1:16:A:GLN:HA  | 3        | 0.12          |
| (1,433) | 1:50:A:MET:HE2  | 1:16:A:GLN:HA  | 3        | 0.12          |
| (1,433) | 1:50:A:MET:HE3  | 1:16:A:GLN:HA  | 3        | 0.12          |
| (1,433) | 1:50:A:MET:HE1  | 1:16:A:GLN:HA  | 6        | 0.12          |
| (1,433) | 1:50:A:MET:HE2  | 1:16:A:GLN:HA  | 6        | 0.12          |
| (1,433) | 1:50:A:MET:HE3  | 1:16:A:GLN:HA  | 6        | 0.12          |
| (1,433) | 1:50:A:MET:HE1  | 1:16:A:GLN:HA  | 15       | 0.12          |
| (1,433) | 1:50:A:MET:HE2  | 1:16:A:GLN:HA  | 15       | 0.12          |
| (1,433) | 1:50:A:MET:HE3  | 1:16:A:GLN:HA  | 15       | 0.12          |
| (1,340) | 1:104:A:PRO:HD2 | 1:8:A:SER:HB2  | 9        | 0.12          |
| (1,340) | 1:104:A:PRO:HD2 | 1:8:A:SER:HB3  | 9        | 0.12          |
| (1,340) | 1:104:A:PRO:HD3 | 1:8:A:SER:HB2  | 9        | 0.12          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,340) | 1:104:A:PRO:HD3 | 1:8:A:SER:HB3  | 9        | 0.12          |
| (1,318) | 1:65:A:ILE:HD11 | 1:7:A:VAL:HG21 | 19       | 0.12          |
| (1,318) | 1:65:A:ILE:HD11 | 1:7:A:VAL:HG22 | 19       | 0.12          |
| (1,318) | 1:65:A:ILE:HD11 | 1:7:A:VAL:HG23 | 19       | 0.12          |
| (1,318) | 1:65:A:ILE:HD12 | 1:7:A:VAL:HG21 | 19       | 0.12          |
| (1,318) | 1:65:A:ILE:HD12 | 1:7:A:VAL:HG22 | 19       | 0.12          |
| (1,318) | 1:65:A:ILE:HD12 | 1:7:A:VAL:HG23 | 19       | 0.12          |
| (1,318) | 1:65:A:ILE:HD13 | 1:7:A:VAL:HG21 | 19       | 0.12          |
| (1,318) | 1:65:A:ILE:HD13 | 1:7:A:VAL:HG22 | 19       | 0.12          |
| (1,318) | 1:65:A:ILE:HD13 | 1:7:A:VAL:HG23 | 19       | 0.12          |
| (1,267) | 1:76:A:VAL:HA   | 1:4:A:VAL:HG21 | 4        | 0.12          |
| (1,267) | 1:76:A:VAL:HA   | 1:4:A:VAL:HG22 | 4        | 0.12          |
| (1,267) | 1:76:A:VAL:HA   | 1:4:A:VAL:HG23 | 4        | 0.12          |
| (1,260) | 1:77:A:ILE:HD11 | 1:4:A:VAL:HG11 | 15       | 0.12          |
| (1,260) | 1:77:A:ILE:HD11 | 1:4:A:VAL:HG12 | 15       | 0.12          |
| (1,260) | 1:77:A:ILE:HD11 | 1:4:A:VAL:HG13 | 15       | 0.12          |
| (1,260) | 1:77:A:ILE:HD12 | 1:4:A:VAL:HG11 | 15       | 0.12          |
| (1,260) | 1:77:A:ILE:HD12 | 1:4:A:VAL:HG12 | 15       | 0.12          |
| (1,260) | 1:77:A:ILE:HD12 | 1:4:A:VAL:HG13 | 15       | 0.12          |
| (1,260) | 1:77:A:ILE:HD13 | 1:4:A:VAL:HG11 | 15       | 0.12          |
| (1,260) | 1:77:A:ILE:HD13 | 1:4:A:VAL:HG12 | 15       | 0.12          |
| (1,260) | 1:77:A:ILE:HD13 | 1:4:A:VAL:HG13 | 15       | 0.12          |
| (1,260) | 1:77:A:ILE:HD11 | 1:4:A:VAL:HG11 | 20       | 0.12          |
| (1,260) | 1:77:A:ILE:HD11 | 1:4:A:VAL:HG12 | 20       | 0.12          |
| (1,260) | 1:77:A:ILE:HD11 | 1:4:A:VAL:HG13 | 20       | 0.12          |
| (1,260) | 1:77:A:ILE:HD12 | 1:4:A:VAL:HG11 | 20       | 0.12          |
| (1,260) | 1:77:A:ILE:HD12 | 1:4:A:VAL:HG12 | 20       | 0.12          |
| (1,260) | 1:77:A:ILE:HD12 | 1:4:A:VAL:HG13 | 20       | 0.12          |
| (1,260) | 1:77:A:ILE:HD13 | 1:4:A:VAL:HG11 | 20       | 0.12          |
| (1,260) | 1:77:A:ILE:HD13 | 1:4:A:VAL:HG12 | 20       | 0.12          |
| (1,260) | 1:77:A:ILE:HD13 | 1:4:A:VAL:HG13 | 20       | 0.12          |
| (1,157) | 1:71:A:ASP:H    | 1:73:A:TYR:HE1 | 2        | 0.12          |
| (1,157) | 1:71:A:ASP:H    | 1:73:A:TYR:HE2 | 2        | 0.12          |
| (1,157) | 1:71:A:ASP:H    | 1:73:A:TYR:HE1 | 4        | 0.12          |
| (1,157) | 1:71:A:ASP:H    | 1:73:A:TYR:HE2 | 4        | 0.12          |
| (1,157) | 1:71:A:ASP:H    | 1:73:A:TYR:HE1 | 8        | 0.12          |
| (1,157) | 1:71:A:ASP:H    | 1:73:A:TYR:HE2 | 8        | 0.12          |
| (1,157) | 1:71:A:ASP:H    | 1:73:A:TYR:HE1 | 13       | 0.12          |
| (1,157) | 1:71:A:ASP:H    | 1:73:A:TYR:HE2 | 13       | 0.12          |
| (1,157) | 1:71:A:ASP:H    | 1:73:A:TYR:HE1 | 16       | 0.12          |
| (1,157) | 1:71:A:ASP:H    | 1:73:A:TYR:HE2 | 16       | 0.12          |
| (1,139) | 1:79:A:LEU:HG   | 1:6:A:PHE:HE1  | 6        | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2   | 6        | 0.12          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1   | 14       | 0.12          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2   | 14       | 0.12          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1   | 18       | 0.12          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2   | 18       | 0.12          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD11 | 15       | 0.12          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD12 | 15       | 0.12          |
| (1,40)   | 1:91:A:VAL:H     | 1:86:A:LEU:HD13 | 15       | 0.12          |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1  | 4        | 0.11          |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1  | 18       | 0.11          |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1  | 20       | 0.11          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1  | 4        | 0.11          |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1  | 4        | 0.11          |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1  | 4        | 0.11          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1  | 7        | 0.11          |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1  | 7        | 0.11          |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1  | 7        | 0.11          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1  | 13       | 0.11          |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1  | 13       | 0.11          |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1  | 13       | 0.11          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1  | 14       | 0.11          |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1  | 14       | 0.11          |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1  | 14       | 0.11          |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1  | 20       | 0.11          |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1  | 20       | 0.11          |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1  | 20       | 0.11          |
| (1,3657) | 1:127:A:ILE:HG12 | 1:127:A:ILE:H   | 7        | 0.11          |
| (1,3657) | 1:127:A:ILE:HG13 | 1:127:A:ILE:H   | 7        | 0.11          |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H   | 12       | 0.11          |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H   | 12       | 0.11          |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H   | 12       | 0.11          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H   | 8        | 0.11          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H   | 8        | 0.11          |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H   | 14       | 0.11          |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H   | 14       | 0.11          |
| (1,3504) | 1:43:A:HIS:HE1   | 1:105:A:ASP:H   | 3        | 0.11          |
| (1,3504) | 1:43:A:HIS:HE1   | 1:105:A:ASP:H   | 8        | 0.11          |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H    | 7        | 0.11          |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H    | 7        | 0.11          |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H    | 11       | 0.11          |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H    | 11       | 0.11          |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H    | 13       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H     | 13       | 0.11          |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H     | 14       | 0.11          |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H     | 14       | 0.11          |
| (1,3080) | 1:10:A:ARG:HA    | 1:40:A:SER:H     | 8        | 0.11          |
| (1,3033) | 1:112:A:PHE:HB2  | 1:106:A:GLY:H    | 7        | 0.11          |
| (1,3033) | 1:112:A:PHE:HB3  | 1:106:A:GLY:H    | 7        | 0.11          |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H     | 16       | 0.11          |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H     | 16       | 0.11          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H     | 10       | 0.11          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H     | 10       | 0.11          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H     | 11       | 0.11          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H     | 11       | 0.11          |
| (1,2995) | 1:29:A:LYS:HD2   | 1:30:A:ILE:H     | 16       | 0.11          |
| (1,2995) | 1:29:A:LYS:HD3   | 1:30:A:ILE:H     | 16       | 0.11          |
| (1,2956) | 1:60:A:GLN:HE21  | 1:24:A:THR:H     | 7        | 0.11          |
| (1,2956) | 1:60:A:GLN:HE22  | 1:24:A:THR:H     | 7        | 0.11          |
| (1,2865) | 1:35:A:SER:HA    | 1:8:A:SER:H      | 10       | 0.11          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2   | 20       | 0.11          |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3   | 20       | 0.11          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2   | 20       | 0.11          |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3   | 20       | 0.11          |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB1  | 12       | 0.11          |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB2  | 12       | 0.11          |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB3  | 12       | 0.11          |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB1  | 17       | 0.11          |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB2  | 17       | 0.11          |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB3  | 17       | 0.11          |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB1  | 18       | 0.11          |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB2  | 18       | 0.11          |
| (1,2694) | 1:125:A:ASN:H    | 1:128:A:ALA:HB3  | 18       | 0.11          |
| (1,2673) | 1:127:A:ILE:H    | 1:127:A:ILE:HG12 | 7        | 0.11          |
| (1,2673) | 1:127:A:ILE:H    | 1:127:A:ILE:HG13 | 7        | 0.11          |
| (1,2653) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HB   | 15       | 0.11          |
| (1,2653) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HB   | 15       | 0.11          |
| (1,2653) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HB   | 15       | 0.11          |
| (1,2649) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HA   | 2        | 0.11          |
| (1,2649) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HA   | 2        | 0.11          |
| (1,2649) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HA   | 2        | 0.11          |
| (1,2546) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HA   | 20       | 0.11          |
| (1,2546) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HA   | 20       | 0.11          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 5        | 0.11          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 5        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 5        | 0.11          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD11 | 9        | 0.11          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD12 | 9        | 0.11          |
| (1,2418) | 1:99:A:TRP:HZ2   | 1:126:A:LEU:HD13 | 9        | 0.11          |
| (1,2094) | 1:115:A:VAL:HG11 | 1:103:A:ASP:HA   | 19       | 0.11          |
| (1,2094) | 1:115:A:VAL:HG12 | 1:103:A:ASP:HA   | 19       | 0.11          |
| (1,2094) | 1:115:A:VAL:HG13 | 1:103:A:ASP:HA   | 19       | 0.11          |
| (1,1980) | 1:91:A:VAL:H     | 1:96:A:PHE:HB2   | 6        | 0.11          |
| (1,1980) | 1:91:A:VAL:H     | 1:96:A:PHE:HB3   | 6        | 0.11          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2   | 7        | 0.11          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3   | 7        | 0.11          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2   | 14       | 0.11          |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3   | 14       | 0.11          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG11  | 9        | 0.11          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG12  | 9        | 0.11          |
| (1,1761) | 1:82:A:CYS:H     | 1:84:A:VAL:HG13  | 9        | 0.11          |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB2   | 4        | 0.11          |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB3   | 4        | 0.11          |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB2   | 11       | 0.11          |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB3   | 11       | 0.11          |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB2   | 8        | 0.11          |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB3   | 8        | 0.11          |
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB2   | 8        | 0.11          |
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB3   | 8        | 0.11          |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB2   | 12       | 0.11          |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB3   | 12       | 0.11          |
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB2   | 12       | 0.11          |
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB3   | 12       | 0.11          |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB2   | 15       | 0.11          |
| (1,1364) | 1:60:A:GLN:HB2   | 1:58:A:SER:HB3   | 15       | 0.11          |
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB2   | 15       | 0.11          |
| (1,1364) | 1:60:A:GLN:HB3   | 1:58:A:SER:HB3   | 15       | 0.11          |
| (1,1355) | 1:47:A:ILE:HG21  | 1:58:A:SER:HA    | 4        | 0.11          |
| (1,1355) | 1:47:A:ILE:HG22  | 1:58:A:SER:HA    | 4        | 0.11          |
| (1,1355) | 1:47:A:ILE:HG23  | 1:58:A:SER:HA    | 4        | 0.11          |
| (1,1355) | 1:47:A:ILE:HG21  | 1:58:A:SER:HA    | 6        | 0.11          |
| (1,1355) | 1:47:A:ILE:HG22  | 1:58:A:SER:HA    | 6        | 0.11          |
| (1,1355) | 1:47:A:ILE:HG23  | 1:58:A:SER:HA    | 6        | 0.11          |
| (1,1355) | 1:47:A:ILE:HG21  | 1:58:A:SER:HA    | 11       | 0.11          |
| (1,1355) | 1:47:A:ILE:HG22  | 1:58:A:SER:HA    | 11       | 0.11          |
| (1,1355) | 1:47:A:ILE:HG23  | 1:58:A:SER:HA    | 11       | 0.11          |
| (1,1340) | 1:41:A:ARG:HG2   | 1:57:A:ILE:HD11  | 17       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1340) | 1:41:A:ARG:HG2 | 1:57:A:ILE:HD12 | 17       | 0.11          |
| (1,1340) | 1:41:A:ARG:HG2 | 1:57:A:ILE:HD13 | 17       | 0.11          |
| (1,1340) | 1:41:A:ARG:HG3 | 1:57:A:ILE:HD11 | 17       | 0.11          |
| (1,1340) | 1:41:A:ARG:HG3 | 1:57:A:ILE:HD12 | 17       | 0.11          |
| (1,1340) | 1:41:A:ARG:HG3 | 1:57:A:ILE:HD13 | 17       | 0.11          |
| (1,1253) | 1:24:A:THR:HB  | 1:54:A:GLY:HA2  | 9        | 0.11          |
| (1,1253) | 1:24:A:THR:HB  | 1:54:A:GLY:HA3  | 9        | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB1  | 6        | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB2  | 6        | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB3  | 6        | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB1  | 6        | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB2  | 6        | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB3  | 6        | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB1  | 7        | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB2  | 7        | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB3  | 7        | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB1  | 7        | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB2  | 7        | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB3  | 7        | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB1  | 11       | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB2  | 11       | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB3  | 11       | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB1  | 11       | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB2  | 11       | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB3  | 11       | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB1  | 14       | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB2  | 14       | 0.11          |
| (1,1133) | 1:50:A:MET:HG2 | 1:48:A:ALA:HB3  | 14       | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB1  | 14       | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB2  | 14       | 0.11          |
| (1,1133) | 1:50:A:MET:HG3 | 1:48:A:ALA:HB3  | 14       | 0.11          |
| (1,991)  | 1:57:A:ILE:H   | 1:42:A:VAL:HB   | 2        | 0.11          |
| (1,991)  | 1:57:A:ILE:H   | 1:42:A:VAL:HB   | 11       | 0.11          |
| (1,991)  | 1:57:A:ILE:H   | 1:42:A:VAL:HB   | 18       | 0.11          |
| (1,928)  | 1:40:A:SER:HA  | 1:38:A:GLU:HA   | 1        | 0.11          |
| (1,928)  | 1:40:A:SER:HA  | 1:38:A:GLU:HA   | 6        | 0.11          |
| (1,928)  | 1:40:A:SER:HA  | 1:38:A:GLU:HA   | 7        | 0.11          |
| (1,928)  | 1:40:A:SER:HA  | 1:38:A:GLU:HA   | 9        | 0.11          |
| (1,877)  | 1:5:A:MET:HG2  | 1:36:A:GLY:HA2  | 1        | 0.11          |
| (1,877)  | 1:5:A:MET:HG2  | 1:36:A:GLY:HA3  | 1        | 0.11          |
| (1,877)  | 1:5:A:MET:HG3  | 1:36:A:GLY:HA2  | 1        | 0.11          |
| (1,877)  | 1:5:A:MET:HG3  | 1:36:A:GLY:HA3  | 1        | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA2  | 5        | 0.11          |
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA3  | 5        | 0.11          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA2  | 5        | 0.11          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA3  | 5        | 0.11          |
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA2  | 12       | 0.11          |
| (1,877) | 1:5:A:MET:HG2  | 1:36:A:GLY:HA3  | 12       | 0.11          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA2  | 12       | 0.11          |
| (1,877) | 1:5:A:MET:HG3  | 1:36:A:GLY:HA3  | 12       | 0.11          |
| (1,849) | 1:6:A:PHE:HE1  | 1:34:A:SER:HA   | 7        | 0.11          |
| (1,849) | 1:6:A:PHE:HE2  | 1:34:A:SER:HA   | 7        | 0.11          |
| (1,826) | 1:5:A:MET:HA   | 1:33:A:THR:HA   | 3        | 0.11          |
| (1,826) | 1:5:A:MET:HA   | 1:33:A:THR:HA   | 10       | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG21 | 1        | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG22 | 1        | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG23 | 1        | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG21 | 1        | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG22 | 1        | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG23 | 1        | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG21 | 6        | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG22 | 6        | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG23 | 6        | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG21 | 6        | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG22 | 6        | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG23 | 6        | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG21 | 15       | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG22 | 15       | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG23 | 15       | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG21 | 15       | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG22 | 15       | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG23 | 15       | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG21 | 18       | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG22 | 18       | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG23 | 18       | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG21 | 18       | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG22 | 18       | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG23 | 18       | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG21 | 19       | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG22 | 19       | 0.11          |
| (1,823) | 1:23:A:LYS:HG2 | 1:32:A:VAL:HG23 | 19       | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG21 | 19       | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG22 | 19       | 0.11          |
| (1,823) | 1:23:A:LYS:HG3 | 1:32:A:VAL:HG23 | 19       | 0.11          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,802) | 1:33:A:THR:HA    | 1:32:A:VAL:HG11 | 19       | 0.11          |
| (1,802) | 1:33:A:THR:HA    | 1:32:A:VAL:HG12 | 19       | 0.11          |
| (1,802) | 1:33:A:THR:HA    | 1:32:A:VAL:HG13 | 19       | 0.11          |
| (1,744) | 1:1:A:MET:HB2    | 1:30:A:ILE:HB   | 14       | 0.11          |
| (1,744) | 1:1:A:MET:HB3    | 1:30:A:ILE:HB   | 14       | 0.11          |
| (1,744) | 1:1:A:MET:HB2    | 1:30:A:ILE:HB   | 19       | 0.11          |
| (1,744) | 1:1:A:MET:HB3    | 1:30:A:ILE:HB   | 19       | 0.11          |
| (1,649) | 1:24:A:THR:HG21  | 1:25:A:LEU:HA   | 1        | 0.11          |
| (1,649) | 1:24:A:THR:HG22  | 1:25:A:LEU:HA   | 1        | 0.11          |
| (1,649) | 1:24:A:THR:HG23  | 1:25:A:LEU:HA   | 1        | 0.11          |
| (1,649) | 1:24:A:THR:HG21  | 1:25:A:LEU:HA   | 6        | 0.11          |
| (1,649) | 1:24:A:THR:HG22  | 1:25:A:LEU:HA   | 6        | 0.11          |
| (1,649) | 1:24:A:THR:HG23  | 1:25:A:LEU:HA   | 6        | 0.11          |
| (1,649) | 1:24:A:THR:HG21  | 1:25:A:LEU:HA   | 8        | 0.11          |
| (1,649) | 1:24:A:THR:HG22  | 1:25:A:LEU:HA   | 8        | 0.11          |
| (1,649) | 1:24:A:THR:HG23  | 1:25:A:LEU:HA   | 8        | 0.11          |
| (1,649) | 1:24:A:THR:HG21  | 1:25:A:LEU:HA   | 9        | 0.11          |
| (1,649) | 1:24:A:THR:HG22  | 1:25:A:LEU:HA   | 9        | 0.11          |
| (1,649) | 1:24:A:THR:HG23  | 1:25:A:LEU:HA   | 9        | 0.11          |
| (1,649) | 1:24:A:THR:HG21  | 1:25:A:LEU:HA   | 13       | 0.11          |
| (1,649) | 1:24:A:THR:HG22  | 1:25:A:LEU:HA   | 13       | 0.11          |
| (1,649) | 1:24:A:THR:HG23  | 1:25:A:LEU:HA   | 13       | 0.11          |
| (1,649) | 1:24:A:THR:HG21  | 1:25:A:LEU:HA   | 15       | 0.11          |
| (1,649) | 1:24:A:THR:HG22  | 1:25:A:LEU:HA   | 15       | 0.11          |
| (1,649) | 1:24:A:THR:HG23  | 1:25:A:LEU:HA   | 15       | 0.11          |
| (1,649) | 1:24:A:THR:HG21  | 1:25:A:LEU:HA   | 16       | 0.11          |
| (1,649) | 1:24:A:THR:HG22  | 1:25:A:LEU:HA   | 16       | 0.11          |
| (1,649) | 1:24:A:THR:HG23  | 1:25:A:LEU:HA   | 16       | 0.11          |
| (1,649) | 1:24:A:THR:HG21  | 1:25:A:LEU:HA   | 19       | 0.11          |
| (1,649) | 1:24:A:THR:HG22  | 1:25:A:LEU:HA   | 19       | 0.11          |
| (1,649) | 1:24:A:THR:HG23  | 1:25:A:LEU:HA   | 19       | 0.11          |
| (1,634) | 1:24:A:THR:H     | 1:24:A:THR:HB   | 10       | 0.11          |
| (1,634) | 1:24:A:THR:H     | 1:24:A:THR:HB   | 18       | 0.11          |
| (1,633) | 1:62:A:SER:HA    | 1:61:A:THR:HB   | 10       | 0.11          |
| (1,480) | 1:119:A:VAL:HG11 | 1:17:A:MET:HG2  | 1        | 0.11          |
| (1,480) | 1:119:A:VAL:HG11 | 1:17:A:MET:HG3  | 1        | 0.11          |
| (1,480) | 1:119:A:VAL:HG12 | 1:17:A:MET:HG2  | 1        | 0.11          |
| (1,480) | 1:119:A:VAL:HG12 | 1:17:A:MET:HG3  | 1        | 0.11          |
| (1,480) | 1:119:A:VAL:HG13 | 1:17:A:MET:HG2  | 1        | 0.11          |
| (1,480) | 1:119:A:VAL:HG13 | 1:17:A:MET:HG3  | 1        | 0.11          |
| (1,480) | 1:119:A:VAL:HG11 | 1:17:A:MET:HG2  | 20       | 0.11          |
| (1,480) | 1:119:A:VAL:HG11 | 1:17:A:MET:HG3  | 20       | 0.11          |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,480) | 1:119:A:VAL:HG12 | 1:17:A:MET:HG2 | 20       | 0.11          |
| (1,480) | 1:119:A:VAL:HG12 | 1:17:A:MET:HG3 | 20       | 0.11          |
| (1,480) | 1:119:A:VAL:HG13 | 1:17:A:MET:HG2 | 20       | 0.11          |
| (1,480) | 1:119:A:VAL:HG13 | 1:17:A:MET:HG3 | 20       | 0.11          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB2 | 5        | 0.11          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB3 | 5        | 0.11          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB2 | 7        | 0.11          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB3 | 7        | 0.11          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB2 | 9        | 0.11          |
| (1,448) | 1:19:A:GLU:H     | 1:16:A:GLN:HB3 | 9        | 0.11          |
| (1,443) | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB2 | 19       | 0.11          |
| (1,443) | 1:10:A:ARG:HB2   | 1:16:A:GLN:HB3 | 19       | 0.11          |
| (1,443) | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB2 | 19       | 0.11          |
| (1,443) | 1:10:A:ARG:HB3   | 1:16:A:GLN:HB3 | 19       | 0.11          |
| (1,433) | 1:50:A:MET:HE1   | 1:16:A:GLN:HA  | 10       | 0.11          |
| (1,433) | 1:50:A:MET:HE2   | 1:16:A:GLN:HA  | 10       | 0.11          |
| (1,433) | 1:50:A:MET:HE3   | 1:16:A:GLN:HA  | 10       | 0.11          |
| (1,433) | 1:50:A:MET:HE1   | 1:16:A:GLN:HA  | 12       | 0.11          |
| (1,433) | 1:50:A:MET:HE2   | 1:16:A:GLN:HA  | 12       | 0.11          |
| (1,433) | 1:50:A:MET:HE3   | 1:16:A:GLN:HA  | 12       | 0.11          |
| (1,433) | 1:50:A:MET:HE1   | 1:16:A:GLN:HA  | 14       | 0.11          |
| (1,433) | 1:50:A:MET:HE2   | 1:16:A:GLN:HA  | 14       | 0.11          |
| (1,433) | 1:50:A:MET:HE3   | 1:16:A:GLN:HA  | 14       | 0.11          |
| (1,433) | 1:50:A:MET:HE1   | 1:16:A:GLN:HA  | 20       | 0.11          |
| (1,433) | 1:50:A:MET:HE2   | 1:16:A:GLN:HA  | 20       | 0.11          |
| (1,433) | 1:50:A:MET:HE3   | 1:16:A:GLN:HA  | 20       | 0.11          |
| (1,340) | 1:104:A:PRO:HD2  | 1:8:A:SER:HB2  | 6        | 0.11          |
| (1,340) | 1:104:A:PRO:HD2  | 1:8:A:SER:HB3  | 6        | 0.11          |
| (1,340) | 1:104:A:PRO:HD3  | 1:8:A:SER:HB2  | 6        | 0.11          |
| (1,340) | 1:104:A:PRO:HD3  | 1:8:A:SER:HB3  | 6        | 0.11          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG21 | 9        | 0.11          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG22 | 9        | 0.11          |
| (1,267) | 1:76:A:VAL:HA    | 1:4:A:VAL:HG23 | 9        | 0.11          |
| (1,262) | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG21 | 12       | 0.11          |
| (1,262) | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG22 | 12       | 0.11          |
| (1,262) | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG23 | 12       | 0.11          |
| (1,262) | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG21 | 12       | 0.11          |
| (1,262) | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG22 | 12       | 0.11          |
| (1,262) | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG23 | 12       | 0.11          |
| (1,262) | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG21 | 12       | 0.11          |
| (1,262) | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG22 | 12       | 0.11          |
| (1,262) | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG23 | 12       | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,262)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG21  | 15       | 0.11          |
| (1,262)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG22  | 15       | 0.11          |
| (1,262)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG23  | 15       | 0.11          |
| (1,262)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG21  | 15       | 0.11          |
| (1,262)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG22  | 15       | 0.11          |
| (1,262)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG23  | 15       | 0.11          |
| (1,262)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG21  | 15       | 0.11          |
| (1,262)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG22  | 15       | 0.11          |
| (1,262)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG23  | 15       | 0.11          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG11  | 14       | 0.11          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG12  | 14       | 0.11          |
| (1,260)  | 1:77:A:ILE:HD11  | 1:4:A:VAL:HG13  | 14       | 0.11          |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG11  | 14       | 0.11          |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG12  | 14       | 0.11          |
| (1,260)  | 1:77:A:ILE:HD12  | 1:4:A:VAL:HG13  | 14       | 0.11          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG11  | 14       | 0.11          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG12  | 14       | 0.11          |
| (1,260)  | 1:77:A:ILE:HD13  | 1:4:A:VAL:HG13  | 14       | 0.11          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE1  | 6        | 0.11          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE2  | 6        | 0.11          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE1  | 11       | 0.11          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE2  | 11       | 0.11          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE1  | 12       | 0.11          |
| (1,157)  | 1:71:A:ASP:H     | 1:73:A:TYR:HE2  | 12       | 0.11          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE1   | 12       | 0.11          |
| (1,139)  | 1:79:A:LEU:HG    | 1:6:A:PHE:HE2   | 12       | 0.11          |
| (1,87)   | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD1 | 4        | 0.11          |
| (1,87)   | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD2 | 4        | 0.11          |
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD1 | 4        | 0.11          |
| (1,87)   | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD2 | 4        | 0.11          |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD1 | 4        | 0.11          |
| (1,87)   | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD2 | 4        | 0.11          |
| (1,3701) | 1:90:A:TRP:H     | 1:90:A:TRP:HE1  | 1        | 0.1           |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1  | 6        | 0.1           |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1  | 6        | 0.1           |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1  | 6        | 0.1           |
| (1,3695) | 1:79:A:LEU:HD21  | 1:99:A:TRP:HE1  | 12       | 0.1           |
| (1,3695) | 1:79:A:LEU:HD22  | 1:99:A:TRP:HE1  | 12       | 0.1           |
| (1,3695) | 1:79:A:LEU:HD23  | 1:99:A:TRP:HE1  | 12       | 0.1           |
| (1,3666) | 1:130:A:ILE:HD11 | 1:128:A:ALA:H   | 13       | 0.1           |
| (1,3666) | 1:130:A:ILE:HD12 | 1:128:A:ALA:H   | 13       | 0.1           |
| (1,3666) | 1:130:A:ILE:HD13 | 1:128:A:ALA:H   | 13       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3657) | 1:127:A:ILE:HG12 | 1:127:A:ILE:H    | 8        | 0.1           |
| (1,3657) | 1:127:A:ILE:HG13 | 1:127:A:ILE:H    | 8        | 0.1           |
| (1,3657) | 1:127:A:ILE:HG12 | 1:127:A:ILE:H    | 13       | 0.1           |
| (1,3657) | 1:127:A:ILE:HG13 | 1:127:A:ILE:H    | 13       | 0.1           |
| (1,3657) | 1:127:A:ILE:HG12 | 1:127:A:ILE:H    | 17       | 0.1           |
| (1,3657) | 1:127:A:ILE:HG13 | 1:127:A:ILE:H    | 17       | 0.1           |
| (1,3552) | 1:115:A:VAL:HG11 | 1:114:A:THR:H    | 1        | 0.1           |
| (1,3552) | 1:115:A:VAL:HG12 | 1:114:A:THR:H    | 1        | 0.1           |
| (1,3552) | 1:115:A:VAL:HG13 | 1:114:A:THR:H    | 1        | 0.1           |
| (1,3539) | 1:110:A:GLU:HB2  | 1:112:A:PHE:H    | 19       | 0.1           |
| (1,3539) | 1:110:A:GLU:HB3  | 1:112:A:PHE:H    | 19       | 0.1           |
| (1,3504) | 1:43:A:HIS:HE1   | 1:105:A:ASP:H    | 18       | 0.1           |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H     | 4        | 0.1           |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H     | 4        | 0.1           |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H     | 6        | 0.1           |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H     | 6        | 0.1           |
| (1,3171) | 1:49:A:MET:HB2   | 1:53:A:VAL:H     | 18       | 0.1           |
| (1,3171) | 1:49:A:MET:HB3   | 1:53:A:VAL:H     | 18       | 0.1           |
| (1,3092) | 1:42:A:VAL:HB    | 1:42:A:VAL:H     | 20       | 0.1           |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H     | 6        | 0.1           |
| (1,3081) | 1:64:A:PRO:HA    | 1:40:A:SER:H     | 20       | 0.1           |
| (1,3033) | 1:112:A:PHE:HB2  | 1:106:A:GLY:H    | 1        | 0.1           |
| (1,3033) | 1:112:A:PHE:HB3  | 1:106:A:GLY:H    | 1        | 0.1           |
| (1,3033) | 1:112:A:PHE:HB2  | 1:106:A:GLY:H    | 12       | 0.1           |
| (1,3033) | 1:112:A:PHE:HB3  | 1:106:A:GLY:H    | 12       | 0.1           |
| (1,3007) | 1:127:A:ILE:HG12 | 1:32:A:VAL:H     | 13       | 0.1           |
| (1,3007) | 1:127:A:ILE:HG13 | 1:32:A:VAL:H     | 13       | 0.1           |
| (1,2939) | 1:60:A:GLN:HE21  | 1:22:A:ALA:H     | 13       | 0.1           |
| (1,2939) | 1:60:A:GLN:HE22  | 1:22:A:ALA:H     | 13       | 0.1           |
| (1,2865) | 1:35:A:SER:HA    | 1:8:A:SER:H      | 5        | 0.1           |
| (1,2865) | 1:35:A:SER:HA    | 1:8:A:SER:H      | 6        | 0.1           |
| (1,2865) | 1:35:A:SER:HA    | 1:8:A:SER:H      | 8        | 0.1           |
| (1,2865) | 1:35:A:SER:HA    | 1:8:A:SER:H      | 12       | 0.1           |
| (1,2865) | 1:35:A:SER:HA    | 1:8:A:SER:H      | 15       | 0.1           |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB2   | 8        | 0.1           |
| (1,2780) | 1:17:A:MET:HB2   | 1:79:A:LEU:HB3   | 8        | 0.1           |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB2   | 8        | 0.1           |
| (1,2780) | 1:17:A:MET:HB3   | 1:79:A:LEU:HB3   | 8        | 0.1           |
| (1,2745) | 1:79:A:LEU:HG    | 1:15:A:SER:HA    | 15       | 0.1           |
| (1,2673) | 1:127:A:ILE:H    | 1:127:A:ILE:HG12 | 8        | 0.1           |
| (1,2673) | 1:127:A:ILE:H    | 1:127:A:ILE:HG13 | 8        | 0.1           |
| (1,2673) | 1:127:A:ILE:H    | 1:127:A:ILE:HG12 | 13       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2673) | 1:127:A:ILE:H    | 1:127:A:ILE:HG13 | 13       | 0.1           |
| (1,2673) | 1:127:A:ILE:H    | 1:127:A:ILE:HG12 | 17       | 0.1           |
| (1,2673) | 1:127:A:ILE:H    | 1:127:A:ILE:HG13 | 17       | 0.1           |
| (1,2653) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HB   | 2        | 0.1           |
| (1,2653) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HB   | 2        | 0.1           |
| (1,2653) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HB   | 2        | 0.1           |
| (1,2653) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HB   | 17       | 0.1           |
| (1,2653) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HB   | 17       | 0.1           |
| (1,2653) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HB   | 17       | 0.1           |
| (1,2649) | 1:126:A:LEU:HD21 | 1:127:A:ILE:HA   | 17       | 0.1           |
| (1,2649) | 1:126:A:LEU:HD22 | 1:127:A:ILE:HA   | 17       | 0.1           |
| (1,2649) | 1:126:A:LEU:HD23 | 1:127:A:ILE:HA   | 17       | 0.1           |
| (1,2546) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HA   | 1        | 0.1           |
| (1,2546) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HA   | 1        | 0.1           |
| (1,2546) | 1:6:A:PHE:HD1    | 1:123:A:VAL:HA   | 16       | 0.1           |
| (1,2546) | 1:6:A:PHE:HD2    | 1:123:A:VAL:HA   | 16       | 0.1           |
| (1,2144) | 1:10:A:ARG:HB2   | 1:104:A:PRO:HD2  | 18       | 0.1           |
| (1,2144) | 1:10:A:ARG:HB2   | 1:104:A:PRO:HD3  | 18       | 0.1           |
| (1,2144) | 1:10:A:ARG:HB3   | 1:104:A:PRO:HD2  | 18       | 0.1           |
| (1,2144) | 1:10:A:ARG:HB3   | 1:104:A:PRO:HD3  | 18       | 0.1           |
| (1,2088) | 1:100:A:GLN:HG2  | 1:101:A:LEU:HG   | 13       | 0.1           |
| (1,2088) | 1:100:A:GLN:HG3  | 1:101:A:LEU:HG   | 13       | 0.1           |
| (1,2088) | 1:100:A:GLN:HG2  | 1:101:A:LEU:HG   | 20       | 0.1           |
| (1,2088) | 1:100:A:GLN:HG3  | 1:101:A:LEU:HG   | 20       | 0.1           |
| (1,1980) | 1:91:A:VAL:H     | 1:96:A:PHE:HB2   | 1        | 0.1           |
| (1,1980) | 1:91:A:VAL:H     | 1:96:A:PHE:HB3   | 1        | 0.1           |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2   | 3        | 0.1           |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3   | 3        | 0.1           |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2   | 11       | 0.1           |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3   | 11       | 0.1           |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2   | 13       | 0.1           |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3   | 13       | 0.1           |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG2   | 16       | 0.1           |
| (1,1943) | 1:93:A:GLN:HA    | 1:94:A:GLU:HG3   | 16       | 0.1           |
| (1,1848) | 1:90:A:TRP:HD1   | 1:89:A:GLU:HG2   | 16       | 0.1           |
| (1,1848) | 1:90:A:TRP:HD1   | 1:89:A:GLU:HG3   | 16       | 0.1           |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB2   | 1        | 0.1           |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB3   | 1        | 0.1           |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB2   | 12       | 0.1           |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB3   | 12       | 0.1           |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB2   | 14       | 0.1           |
| (1,1366) | 1:47:A:ILE:H     | 1:58:A:SER:HB3   | 14       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1366) | 1:47:A:ILE:H    | 1:58:A:SER:HB2  | 18       | 0.1           |
| (1,1366) | 1:47:A:ILE:H    | 1:58:A:SER:HB3  | 18       | 0.1           |
| (1,1364) | 1:60:A:GLN:HB2  | 1:58:A:SER:HB2  | 16       | 0.1           |
| (1,1364) | 1:60:A:GLN:HB2  | 1:58:A:SER:HB3  | 16       | 0.1           |
| (1,1364) | 1:60:A:GLN:HB3  | 1:58:A:SER:HB2  | 16       | 0.1           |
| (1,1364) | 1:60:A:GLN:HB3  | 1:58:A:SER:HB3  | 16       | 0.1           |
| (1,1355) | 1:47:A:ILE:HG21 | 1:58:A:SER:HA   | 13       | 0.1           |
| (1,1355) | 1:47:A:ILE:HG22 | 1:58:A:SER:HA   | 13       | 0.1           |
| (1,1355) | 1:47:A:ILE:HG23 | 1:58:A:SER:HA   | 13       | 0.1           |
| (1,1253) | 1:24:A:THR:HB   | 1:54:A:GLY:HA2  | 1        | 0.1           |
| (1,1253) | 1:24:A:THR:HB   | 1:54:A:GLY:HA3  | 1        | 0.1           |
| (1,1133) | 1:50:A:MET:HG2  | 1:48:A:ALA:HB1  | 2        | 0.1           |
| (1,1133) | 1:50:A:MET:HG2  | 1:48:A:ALA:HB2  | 2        | 0.1           |
| (1,1133) | 1:50:A:MET:HG2  | 1:48:A:ALA:HB3  | 2        | 0.1           |
| (1,1133) | 1:50:A:MET:HG3  | 1:48:A:ALA:HB1  | 2        | 0.1           |
| (1,1133) | 1:50:A:MET:HG3  | 1:48:A:ALA:HB2  | 2        | 0.1           |
| (1,1133) | 1:50:A:MET:HG3  | 1:48:A:ALA:HB3  | 2        | 0.1           |
| (1,1075) | 1:112:A:PHE:HB2 | 1:46:A:ALA:HB1  | 2        | 0.1           |
| (1,1075) | 1:112:A:PHE:HB2 | 1:46:A:ALA:HB2  | 2        | 0.1           |
| (1,1075) | 1:112:A:PHE:HB2 | 1:46:A:ALA:HB3  | 2        | 0.1           |
| (1,1075) | 1:112:A:PHE:HB3 | 1:46:A:ALA:HB1  | 2        | 0.1           |
| (1,1075) | 1:112:A:PHE:HB3 | 1:46:A:ALA:HB2  | 2        | 0.1           |
| (1,1075) | 1:112:A:PHE:HB3 | 1:46:A:ALA:HB3  | 2        | 0.1           |
| (1,992)  | 1:42:A:VAL:H    | 1:42:A:VAL:HB   | 20       | 0.1           |
| (1,991)  | 1:57:A:ILE:H    | 1:42:A:VAL:HB   | 4        | 0.1           |
| (1,928)  | 1:40:A:SER:HA   | 1:38:A:GLU:HA   | 4        | 0.1           |
| (1,849)  | 1:6:A:PHE:HE1   | 1:34:A:SER:HA   | 10       | 0.1           |
| (1,849)  | 1:6:A:PHE:HE2   | 1:34:A:SER:HA   | 10       | 0.1           |
| (1,823)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG21 | 7        | 0.1           |
| (1,823)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG22 | 7        | 0.1           |
| (1,823)  | 1:23:A:LYS:HG2  | 1:32:A:VAL:HG23 | 7        | 0.1           |
| (1,823)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG21 | 7        | 0.1           |
| (1,823)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG22 | 7        | 0.1           |
| (1,823)  | 1:23:A:LYS:HG3  | 1:32:A:VAL:HG23 | 7        | 0.1           |
| (1,802)  | 1:33:A:THR:HA   | 1:32:A:VAL:HG11 | 20       | 0.1           |
| (1,802)  | 1:33:A:THR:HA   | 1:32:A:VAL:HG12 | 20       | 0.1           |
| (1,802)  | 1:33:A:THR:HA   | 1:32:A:VAL:HG13 | 20       | 0.1           |
| (1,712)  | 1:4:A:VAL:HG21  | 1:75:A:VAL:HB   | 6        | 0.1           |
| (1,712)  | 1:4:A:VAL:HG22  | 1:75:A:VAL:HB   | 6        | 0.1           |
| (1,712)  | 1:4:A:VAL:HG23  | 1:75:A:VAL:HB   | 6        | 0.1           |
| (1,649)  | 1:24:A:THR:HG21 | 1:25:A:LEU:HA   | 12       | 0.1           |
| (1,649)  | 1:24:A:THR:HG22 | 1:25:A:LEU:HA   | 12       | 0.1           |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,649) | 1:24:A:THR:HG23  | 1:25:A:LEU:HA   | 12       | 0.1           |
| (1,633) | 1:62:A:SER:HA    | 1:61:A:THR:HB   | 20       | 0.1           |
| (1,486) | 1:123:A:VAL:HA   | 1:18:A:ALA:HA   | 2        | 0.1           |
| (1,486) | 1:123:A:VAL:HA   | 1:18:A:ALA:HA   | 4        | 0.1           |
| (1,486) | 1:123:A:VAL:HA   | 1:18:A:ALA:HA   | 19       | 0.1           |
| (1,480) | 1:119:A:VAL:HG11 | 1:17:A:MET:HG2  | 6        | 0.1           |
| (1,480) | 1:119:A:VAL:HG11 | 1:17:A:MET:HG3  | 6        | 0.1           |
| (1,480) | 1:119:A:VAL:HG12 | 1:17:A:MET:HG2  | 6        | 0.1           |
| (1,480) | 1:119:A:VAL:HG12 | 1:17:A:MET:HG3  | 6        | 0.1           |
| (1,480) | 1:119:A:VAL:HG13 | 1:17:A:MET:HG2  | 6        | 0.1           |
| (1,480) | 1:119:A:VAL:HG13 | 1:17:A:MET:HG3  | 6        | 0.1           |
| (1,480) | 1:119:A:VAL:HG11 | 1:17:A:MET:HG2  | 14       | 0.1           |
| (1,480) | 1:119:A:VAL:HG11 | 1:17:A:MET:HG3  | 14       | 0.1           |
| (1,480) | 1:119:A:VAL:HG12 | 1:17:A:MET:HG2  | 14       | 0.1           |
| (1,480) | 1:119:A:VAL:HG12 | 1:17:A:MET:HG3  | 14       | 0.1           |
| (1,480) | 1:119:A:VAL:HG13 | 1:17:A:MET:HG2  | 14       | 0.1           |
| (1,480) | 1:119:A:VAL:HG13 | 1:17:A:MET:HG3  | 14       | 0.1           |
| (1,433) | 1:50:A:MET:HE1   | 1:16:A:GLN:HA   | 4        | 0.1           |
| (1,433) | 1:50:A:MET:HE2   | 1:16:A:GLN:HA   | 4        | 0.1           |
| (1,433) | 1:50:A:MET:HE3   | 1:16:A:GLN:HA   | 4        | 0.1           |
| (1,157) | 1:71:A:ASP:H     | 1:73:A:TYR:HE1  | 1        | 0.1           |
| (1,157) | 1:71:A:ASP:H     | 1:73:A:TYR:HE2  | 1        | 0.1           |
| (1,157) | 1:71:A:ASP:H     | 1:73:A:TYR:HE1  | 3        | 0.1           |
| (1,157) | 1:71:A:ASP:H     | 1:73:A:TYR:HE2  | 3        | 0.1           |
| (1,102) | 1:89:A:GLU:HG2   | 1:90:A:TRP:HD1  | 16       | 0.1           |
| (1,102) | 1:89:A:GLU:HG3   | 1:90:A:TRP:HD1  | 16       | 0.1           |
| (1,87)  | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD1 | 10       | 0.1           |
| (1,87)  | 1:115:A:VAL:HG11 | 1:112:A:PHE:HD2 | 10       | 0.1           |
| (1,87)  | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD1 | 10       | 0.1           |
| (1,87)  | 1:115:A:VAL:HG12 | 1:112:A:PHE:HD2 | 10       | 0.1           |
| (1,87)  | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD1 | 10       | 0.1           |
| (1,87)  | 1:115:A:VAL:HG13 | 1:112:A:PHE:HD2 | 10       | 0.1           |
| (1,44)  | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB2  | 5        | 0.1           |
| (1,44)  | 1:86:A:LEU:HD11  | 1:87:A:PRO:HB3  | 5        | 0.1           |
| (1,44)  | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB2  | 5        | 0.1           |
| (1,44)  | 1:86:A:LEU:HD12  | 1:87:A:PRO:HB3  | 5        | 0.1           |
| (1,44)  | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB2  | 5        | 0.1           |
| (1,44)  | 1:86:A:LEU:HD13  | 1:87:A:PRO:HB3  | 5        | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found