



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 3, 2023 – 08:18 PM EDT

PDB ID : 2N0K  
BMRB ID : 25527  
Title : Chemical shift assignments and structure of the alpha-crystallin domain from human, HSPB5  
Authors : Rajagopal, P.; Klevit, R.E.; Shi, L.; Baker, D.  
Deposited on : 2015-03-09

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

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

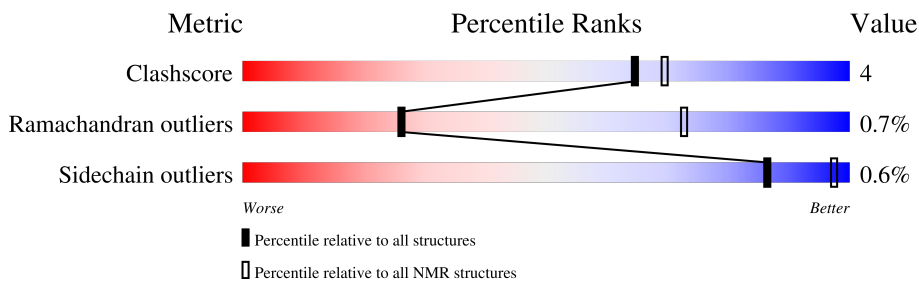
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 43%.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 89     |                  |
| 1   | B     | 89     |                  |

## 2 Ensemble composition and analysis i

This entry contains 9 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:67-A:149, B:67-B:149<br>(166) | 1.50              | 9            |

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 1 clusters and 4 single-model clusters were found.

| Cluster number        | Models        |
|-----------------------|---------------|
| 1                     | 1, 3, 5, 6, 9 |
| Single-model clusters | 2; 4; 7; 8    |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2868 atoms, of which 1432 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-crystallin B chain.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
|     |       |          | Total | C   | H   | N   | O   | S |       |
| 1   | A     | 89       | 1434  | 448 | 716 | 130 | 139 | 1 | 0     |
| 1   | B     | 89       | 1434  | 448 | 716 | 130 | 139 | 1 | 0     |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 146     | ASP      | ASN    | engineered mutation | UNP P02511 |
| B     | 146     | ASP      | ASN    | engineered mutation | UNP P02511 |

## 4 Residue-property plots

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


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

- Molecule 1: Alpha-crystallin B chain

Chain A:  89% 7%



- Molecule 1: Alpha-crystallin B chain

Chain B:  89% 7%




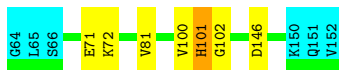
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.


#### 4.2.1 Score per residue for model 1

- Molecule 1: Alpha-crystallin B chain

Chain A:  85% 7% 7%



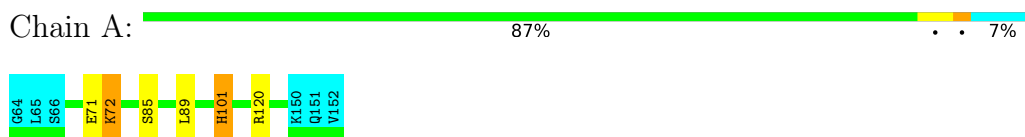
- Molecule 1: Alpha-crystallin B chain

Chain B:  85% 7% 7%

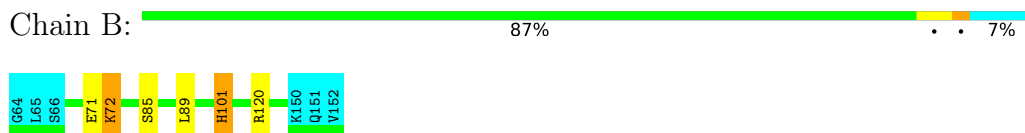


### 4.2.2 Score per residue for model 2

- Molecule 1: Alpha-crystallin B chain

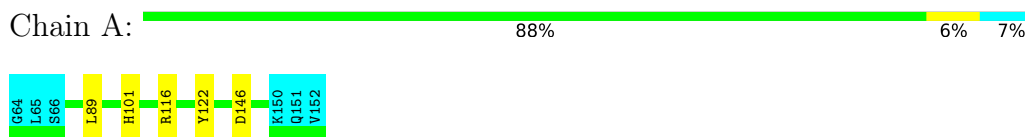


- Molecule 1: Alpha-crystallin B chain

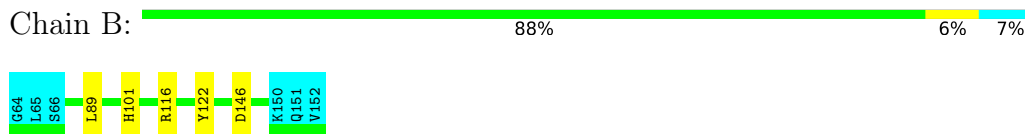


### 4.2.3 Score per residue for model 3

- Molecule 1: Alpha-crystallin B chain

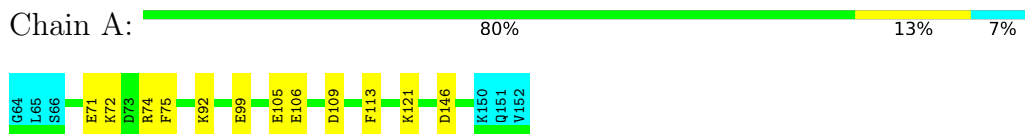


- Molecule 1: Alpha-crystallin B chain

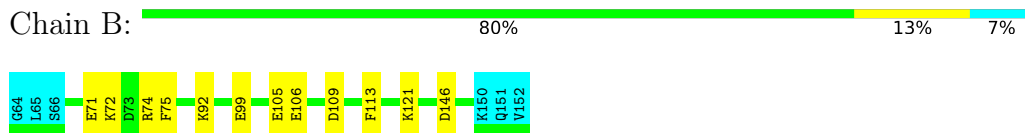


### 4.2.4 Score per residue for model 4

- Molecule 1: Alpha-crystallin B chain

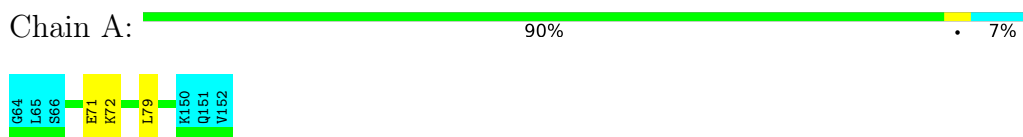


- Molecule 1: Alpha-crystallin B chain

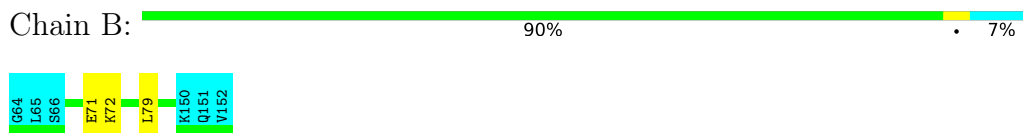


### 4.2.5 Score per residue for model 5

- Molecule 1: Alpha-crystallin B chain

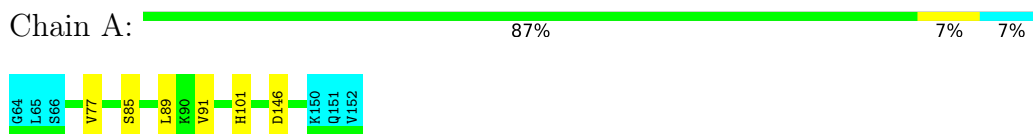


- Molecule 1: Alpha-crystallin B chain

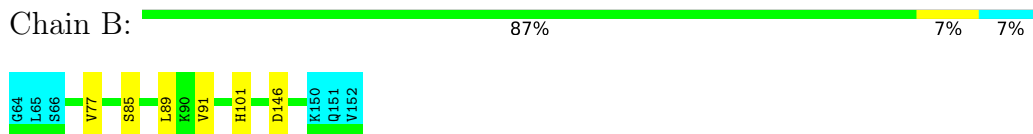


### 4.2.6 Score per residue for model 6

- Molecule 1: Alpha-crystallin B chain

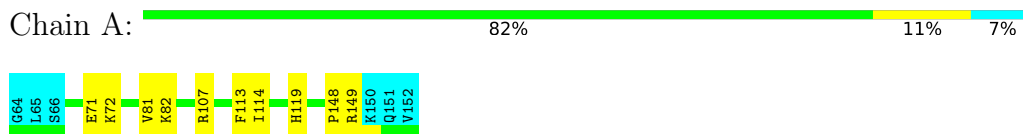


- Molecule 1: Alpha-crystallin B chain

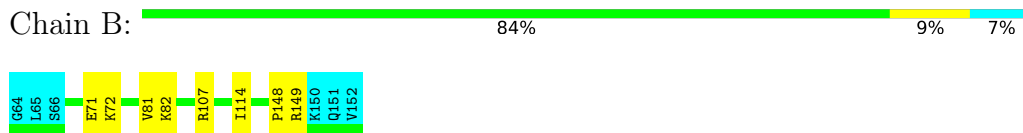


### 4.2.7 Score per residue for model 7

- Molecule 1: Alpha-crystallin B chain

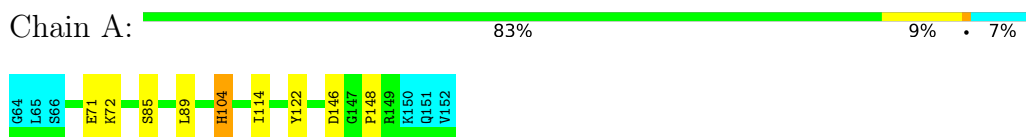


- Molecule 1: Alpha-crystallin B chain

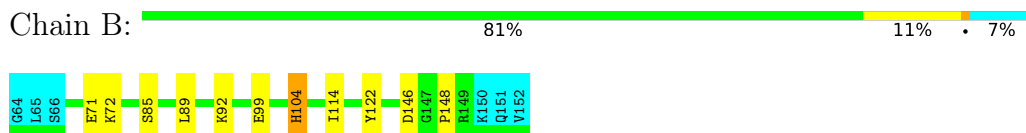


### 4.2.8 Score per residue for model 8

- Molecule 1: Alpha-crystallin B chain

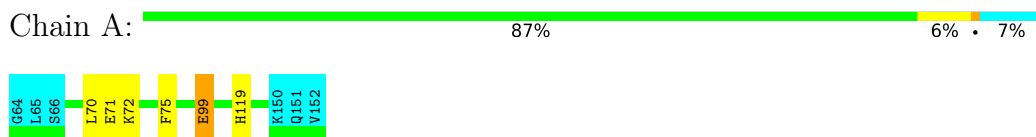


- Molecule 1: Alpha-crystallin B chain

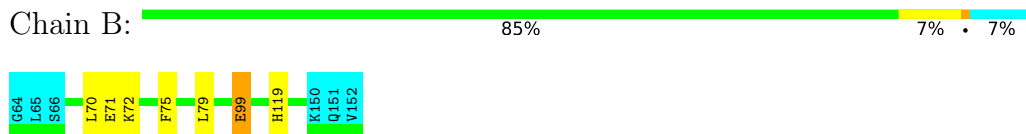


### 4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Alpha-crystallin B chain



- Molecule 1: Alpha-crystallin B chain





## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 9 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 |
|-----------------|--------------------|---------|
| CS-ROSETTA      | structure solution |         |
| RosettaOligomer | structure solution |         |
| TALOS           | refinement         |         |
| RosettaOligomer | refinement         |         |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s)                       | working_cs.cif |
|--|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1075           |
| Number of shifts mapped to atoms             | 1075           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 43%            |

## 6 Model quality i

### 6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts i

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 674   | 665      | 664      | 6±2     |
| 1   | B     | 674   | 665      | 664      | 6±2     |
| All | All   | 12132 | 11970    | 11952    | 102     |

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 4.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:119:HIS:ND1 | 1:B:119:HIS:O   | 0.85     | 2.09        | 9      | 1     |
| 1:A:119:HIS:ND1 | 1:A:119:HIS:O   | 0.83     | 2.09        | 9      | 1     |
| 1:B:146:ASP:O   | 1:B:146:ASP:OD1 | 0.72     | 2.07        | 8      | 2     |
| 1:A:146:ASP:OD1 | 1:A:146:ASP:O   | 0.71     | 2.07        | 8      | 2     |
| 1:B:77:VAL:HG13 | 1:B:77:VAL:O    | 0.67     | 1.89        | 6      | 1     |
| 1:B:81:VAL:HG12 | 1:B:81:VAL:O    | 0.67     | 1.90        | 1      | 2     |
| 1:A:77:VAL:HG13 | 1:A:77:VAL:O    | 0.66     | 1.89        | 6      | 1     |
| 1:B:116:ARG:HG3 | 1:B:116:ARG:O   | 0.66     | 1.90        | 3      | 1     |
| 1:A:81:VAL:O    | 1:A:81:VAL:HG12 | 0.66     | 1.90        | 1      | 2     |
| 1:A:116:ARG:HG3 | 1:A:116:ARG:O   | 0.65     | 1.90        | 3      | 1     |
| 1:B:101:HIS:ND1 | 1:B:101:HIS:O   | 0.64     | 2.31        | 1      | 1     |
| 1:A:71:GLU:O    | 1:A:72:LYS:C    | 0.64     | 2.36        | 2      | 7     |
| 1:A:101:HIS:ND1 | 1:A:101:HIS:O   | 0.63     | 2.31        | 1      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:B:71:GLU:O    | 1:B:72:LYS:C     | 0.62     | 2.36        | 2      | 7     |
| 1:A:99:GLU:HG3  | 1:A:99:GLU:O     | 0.60     | 1.96        | 9      | 1     |
| 1:B:99:GLU:O    | 1:B:99:GLU:HG3   | 0.60     | 1.96        | 9      | 1     |
| 1:A:114:ILE:C   | 1:A:114:ILE:HD12 | 0.58     | 2.18        | 8      | 1     |
| 1:B:114:ILE:C   | 1:B:114:ILE:HD12 | 0.58     | 2.18        | 8      | 1     |
| 1:A:105:GLU:O   | 1:A:106:GLU:C    | 0.57     | 2.43        | 4      | 1     |
| 1:B:105:GLU:O   | 1:B:106:GLU:C    | 0.56     | 2.43        | 4      | 1     |
| 1:A:146:ASP:C   | 1:A:146:ASP:OD1  | 0.55     | 2.45        | 6      | 3     |
| 1:B:101:HIS:CD2 | 1:B:101:HIS:N    | 0.55     | 2.75        | 2      | 1     |
| 1:B:120:ARG:O   | 1:B:120:ARG:CG   | 0.55     | 2.55        | 2      | 1     |
| 1:A:77:VAL:O    | 1:A:77:VAL:CG1   | 0.55     | 2.55        | 6      | 1     |
| 1:B:146:ASP:C   | 1:B:146:ASP:OD1  | 0.54     | 2.45        | 6      | 3     |
| 1:A:120:ARG:CG  | 1:A:120:ARG:O    | 0.54     | 2.55        | 2      | 1     |
| 1:A:75:PHE:O    | 1:A:75:PHE:CD2   | 0.54     | 2.61        | 9      | 1     |
| 1:B:77:VAL:O    | 1:B:77:VAL:CG1   | 0.53     | 2.55        | 6      | 1     |
| 1:A:101:HIS:CD2 | 1:A:101:HIS:N    | 0.53     | 2.75        | 2      | 1     |
| 1:B:75:PHE:O    | 1:B:75:PHE:CD2   | 0.53     | 2.61        | 9      | 1     |
| 1:A:81:VAL:O    | 1:A:82:LYS:C     | 0.50     | 2.50        | 7      | 1     |
| 1:A:113:PHE:O   | 1:B:121:LYS:N    | 0.49     | 2.44        | 4      | 1     |
| 1:B:81:VAL:O    | 1:B:82:LYS:C     | 0.48     | 2.50        | 7      | 1     |
| 1:A:81:VAL:O    | 1:A:81:VAL:CG1   | 0.48     | 2.61        | 1      | 2     |
| 1:B:116:ARG:O   | 1:B:116:ARG:CG   | 0.48     | 2.62        | 3      | 1     |
| 1:A:99:GLU:O    | 1:A:99:GLU:CG    | 0.48     | 2.62        | 9      | 1     |
| 1:A:101:HIS:O   | 1:A:101:HIS:CD2  | 0.48     | 2.67        | 3      | 2     |
| 1:A:121:LYS:N   | 1:B:113:PHE:O    | 0.48     | 2.44        | 4      | 1     |
| 1:B:99:GLU:O    | 1:B:99:GLU:CG    | 0.48     | 2.62        | 9      | 1     |
| 1:B:104:HIS:ND1 | 1:B:104:HIS:C    | 0.47     | 2.67        | 8      | 1     |
| 1:B:119:HIS:O   | 1:B:119:HIS:CG   | 0.47     | 2.67        | 9      | 1     |
| 1:B:101:HIS:O   | 1:B:101:HIS:CD2  | 0.47     | 2.67        | 3      | 2     |
| 1:A:122:TYR:C   | 1:A:122:TYR:CD1  | 0.47     | 2.88        | 3      | 2     |
| 1:A:104:HIS:C   | 1:A:104:HIS:ND1  | 0.47     | 2.67        | 8      | 1     |
| 1:B:122:TYR:CD1 | 1:B:122:TYR:C    | 0.46     | 2.88        | 3      | 2     |
| 1:A:101:HIS:CD2 | 1:A:101:HIS:C    | 0.45     | 2.90        | 6      | 2     |
| 1:A:85:SER:O    | 1:A:89:LEU:N     | 0.45     | 2.50        | 8      | 3     |
| 1:B:85:SER:O    | 1:B:89:LEU:N     | 0.44     | 2.50        | 8      | 3     |
| 1:A:75:PHE:CD1  | 1:A:75:PHE:C     | 0.44     | 2.91        | 4      | 1     |
| 1:B:81:VAL:O    | 1:B:81:VAL:CG1   | 0.44     | 2.65        | 7      | 1     |
| 1:B:101:HIS:CD2 | 1:B:101:HIS:C    | 0.44     | 2.90        | 6      | 2     |
| 1:B:70:LEU:C    | 1:B:70:LEU:HD23  | 0.43     | 2.33        | 9      | 1     |
| 1:B:100:VAL:O   | 1:B:102:GLY:N    | 0.43     | 2.51        | 1      | 1     |
| 1:A:70:LEU:HD23 | 1:A:70:LEU:C     | 0.43     | 2.33        | 9      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:91:VAL:O    | 1:A:91:VAL:HG13  | 0.43     | 2.14        | 6      | 1     |
| 1:B:75:PHE:C    | 1:B:75:PHE:CD1   | 0.42     | 2.91        | 4      | 1     |
| 1:B:91:VAL:O    | 1:B:91:VAL:HG13  | 0.42     | 2.14        | 6      | 1     |
| 1:A:119:HIS:O   | 1:A:119:HIS:CG   | 0.42     | 2.67        | 9      | 2     |
| 1:B:92:LYS:O    | 1:B:99:GLU:N     | 0.42     | 2.52        | 4      | 2     |
| 1:A:100:VAL:O   | 1:A:102:GLY:N    | 0.42     | 2.51        | 1      | 1     |
| 1:A:114:ILE:C   | 1:A:114:ILE:CD1  | 0.42     | 2.88        | 8      | 1     |
| 1:A:71:GLU:N    | 1:A:74:ARG:O     | 0.42     | 2.52        | 4      | 1     |
| 1:A:148:PRO:O   | 1:A:149:ARG:C    | 0.41     | 2.58        | 7      | 1     |
| 1:A:92:LYS:O    | 1:A:99:GLU:N     | 0.41     | 2.52        | 4      | 1     |
| 1:B:148:PRO:O   | 1:B:149:ARG:C    | 0.41     | 2.58        | 7      | 1     |
| 1:B:107:ARG:HB3 | 1:B:114:ILE:HG13 | 0.40     | 1.93        | 7      | 1     |
| 1:B:71:GLU:N    | 1:B:74:ARG:O     | 0.40     | 2.53        | 4      | 1     |
| 1:A:107:ARG:HB3 | 1:A:114:ILE:HG13 | 0.40     | 1.93        | 7      | 1     |
| 1:A:113:PHE:CD1 | 1:A:113:PHE:C    | 0.40     | 2.95        | 7      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed      | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|------------|-------------|----|
| 1   | A     | 83/89 (93%)     | 69±3 (83±3%) | 14±3 (17±3%) | 1±0 (1±1%) | 26          | 73 |
| 1   | B     | 83/89 (93%)     | 69±3 (83±3%) | 14±3 (17±3%) | 1±0 (1±1%) | 26          | 73 |
| All | All   | 1494/1602 (93%) | 1236 (83%)   | 248 (17%)    | 10 (1%)    | 26          | 73 |

All 10 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     | 101 | HIS  | 1              |
| 1   | B     | 101 | HIS  | 1              |
| 1   | A     | 72  | LYS  | 1              |
| 1   | B     | 72  | LYS  | 1              |
| 1   | A     | 109 | ASP  | 1              |
| 1   | B     | 109 | ASP  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 148 | PRO  | 1              |
| 1   | B     | 148 | PRO  | 1              |
| 1   | A     | 99  | GLU  | 1              |
| 1   | B     | 99  | GLU  | 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     | 77/82 (94%)     | 77±0 (99±1%) | 0±0 (1±1%) | 86 97       |
| 1   | B     | 77/82 (94%)     | 76±0 (99±1%) | 1±0 (1±1%) | 84 97       |
| All | All   | 1386/1476 (94%) | 1377 (99%)   | 9 (1%)     | 86 97       |

All 8 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   | B     | 79  | LEU  | 2              |
| 1   | A     | 101 | HIS  | 1              |
| 1   | B     | 101 | HIS  | 1              |
| 1   | A     | 89  | LEU  | 1              |
| 1   | B     | 89  | LEU  | 1              |
| 1   | A     | 79  | LEU  | 1              |
| 1   | A     | 104 | HIS  | 1              |
| 1   | B     | 104 | HIS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 43% for the well-defined parts and 43% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *HSPB5\_ACD\_chemical\_shifts*

#### 7.1.1 Bookkeeping [i](#)

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

|   |      |
|---|------|
| Total number of shifts                  | 1075 |
| Number of shifts mapped to atoms        | 1075 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 4    |

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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action        |
|------------------------|----------|---------------------------------|-------------------------|
| $^{13}\text{C}_\alpha$ | 87       | $-0.01 \pm 0.21$                | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$  | 82       | $0.22 \pm 0.19$                 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$       | 78       | $0.28 \pm 0.15$                 | None needed (< 0.5 ppm) |
| $^{15}\text{N}$        | 81       | $-0.43 \pm 0.42$                | None needed (< 0.5 ppm) |

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 43%, i.e. 1006 atoms were assigned a chemical shift out of a possible 2334. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 400/824 (49%)  | 166/334 (50%) | 156/332 (47%)   | 78/158 (49%)    |
| Sidechain | 543/1336 (41%) | 382/858 (45%) | 159/420 (38%)   | 2/58 (3%)       |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 63/174 (36%)    | 31/88 (35%)    | 22/70 (31%)     | 10/16 (62%)     |
| Overall  | 1006/2334 (43%) | 579/1280 (45%) | 337/822 (41%)   | 90/232 (39%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 1073 atoms were assigned a chemical shift out of a possible 2494. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 421/886 (48%)   | 175/360 (49%)  | 165/356 (46%)   | 81/170 (48%)    |
| Sidechain | 589/1434 (41%)  | 414/922 (45%)  | 172/450 (38%)   | 3/62 (5%)       |
| Aromatic  | 63/174 (36%)    | 31/88 (35%)    | 22/70 (31%)     | 10/16 (62%)     |
| Overall   | 1073/2494 (43%) | 620/1370 (45%) | 359/876 (41%)   | 94/248 (38%)    |

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

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

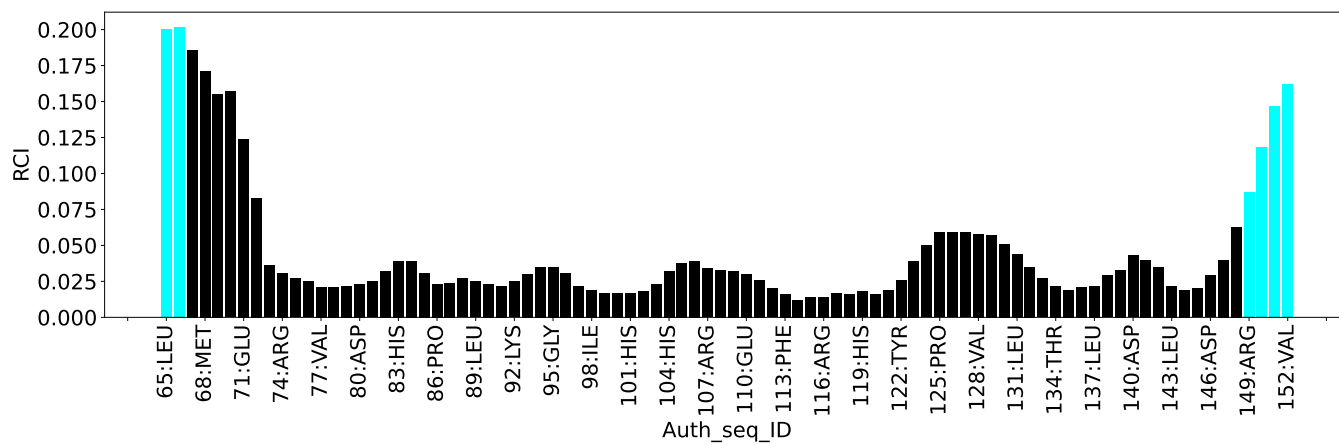
| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 132 | THR  | HG1  | 5.90       | 0.08 – 2.19         | 22.6    |
| 1       | A     | 144 | THR  | HG1  | 5.62       | 0.08 – 2.19         | 21.2    |
| 1       | A     | 94  | LEU  | CG   | 35.67      | 21.37 – 32.19       | 8.2     |
| 1       | A     | 102 | GLY  | HA3  | 1.95       | 2.08 – 5.71         | -5.4    |

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

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

Random coil index (RCI) for chain A:





## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description  | Value |
|--|-------|
| Total distance restraints                                | 1770  |
| Intra-residue ( $ i-j =0$ )                              | 622   |
| Sequential ( $ i-j =1$ )                                 | 512   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 200   |
| Long range ( $ i-j \geq 5$ )                             | 400   |
| Inter-chain  | 36    |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 226   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 11.2  |
| Number of long range restraints per residue <sup>1</sup> | 2.2   |

<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)  | 127.6                                  | 0.2     |
| 0.2-0.5 (Medium) | 261.9                                  | 0.5     |
| >0.5 (Large)     | 358.6                                  | 20.97   |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small)   | 27.4                                   | 9.8     |
| 10.0-20.0 (Medium) | 17.7                                   | 19.8    |
| >20.0 (Large)      | 25.9                                   | 134.6   |

## 9 Distance violation analysis

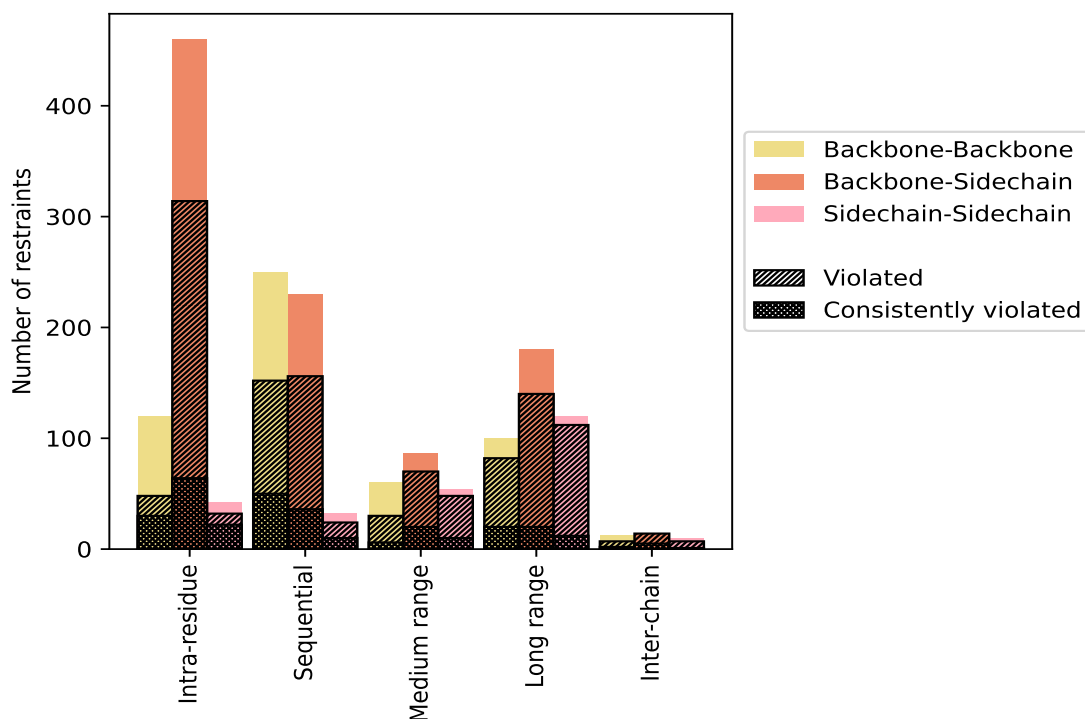
### 9.1 Summary of distance violations

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>622</b>  | <b>35.1</b>    | <b>394</b>            | <b>63.3</b>    | <b>22.3</b>    | <b>116</b>                         | <b>18.6</b>    | <b>6.6</b>     |
| Backbone-Backbone   | 120         | 6.8            | 48                    | 40.0           | 2.7            | 30                                 | 25.0           | 1.7            |
| Backbone-Sidechain  | 460         | 26.0           | 314                   | 68.3           | 17.7           | 64                                 | 13.9           | 3.6            |
| Sidechain-Sidechain   | 42          | 2.4            | 32                    | 76.2           | 1.8            | 22                                 | 52.4           | 1.2            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>512</b>  | <b>28.9</b>    | <b>332</b>            | <b>64.8</b>    | <b>18.8</b>    | <b>96</b>                          | <b>18.8</b>    | <b>5.4</b>     |
| Backbone-Backbone   | 250         | 14.1           | 152                   | 60.8           | 8.6            | 50                                 | 20.0           | 2.8            |
| Backbone-Sidechain  | 230         | 13.0           | 156                   | 67.8           | 8.8            | 36                                 | 15.7           | 2.0            |
| Sidechain-Sidechain   | 32          | 1.8            | 24                    | 75.0           | 1.4            | 10                                 | 31.2           | 0.6            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>200</b>  | <b>11.3</b>    | <b>148</b>            | <b>74.0</b>    | <b>8.4</b>     | <b>36</b>                          | <b>18.0</b>    | <b>2.0</b>     |
| Backbone-Backbone   | 60          | 3.4            | 30                    | 50.0           | 1.7            | 6                                  | 10.0           | 0.3            |
| Backbone-Sidechain  | 86          | 4.9            | 70                    | 81.4           | 4.0            | 20                                 | 23.3           | 1.1            |
| Sidechain-Sidechain   | 54          | 3.1            | 48                    | 88.9           | 2.7            | 10                                 | 18.5           | 0.6            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>400</b>  | <b>22.6</b>    | <b>334</b>            | <b>83.5</b>    | <b>18.9</b>    | <b>52</b>                          | <b>13.0</b>    | <b>2.9</b>     |
| Backbone-Backbone   | 100         | 5.6            | 82                    | 82.0           | 4.6            | 20                                 | 20.0           | 1.1            |
| Backbone-Sidechain  | 180         | 10.2           | 140                   | 77.8           | 7.9            | 20                                 | 11.1           | 1.1            |
| Sidechain-Sidechain   | 120         | 6.8            | 112                   | 93.3           | 6.3            | 12                                 | 10.0           | 0.7            |
| <b>Inter-chain</b>  | <b>36</b>   | <b>2.0</b>     | <b>28</b>             | <b>77.8</b>    | <b>1.6</b>     | <b>8</b>                           | <b>22.2</b>    | <b>0.5</b>     |
| Backbone-Backbone   | 12          | 0.7            | 7                     | 58.3           | 0.4            | 2                                  | 16.7           | 0.1            |
| Backbone-Sidechain  | 14          | 0.8            | 14                    | 100.0          | 0.8            | 5                                  | 35.7           | 0.3            |
| Sidechain-Sidechain   | 10          | 0.6            | 7                     | 70.0           | 0.4            | 1                                  | 10.0           | 0.1            |
| Hydrogen bond   | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Disulfide bond  | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Total</b>  | <b>1770</b> | <b>100.0</b>   | <b>1236</b>           | <b>69.8</b>    | <b>69.8</b>    | <b>308</b>                         | <b>17.4</b>    | <b>17.4</b>    |
| Backbone-Backbone   | 542         | 30.6           | 319                   | 58.9           | 18.0           | 108                                | 19.9           | 6.1            |
| Backbone-Sidechain  | 970         | 54.8           | 694                   | 71.5           | 39.2           | 145                                | 14.9           | 8.2            |
| Sidechain-Sidechain   | 258         | 14.6           | 223                   | 86.4           | 12.6           | 55                                 | 21.3           | 3.1            |

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

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



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

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

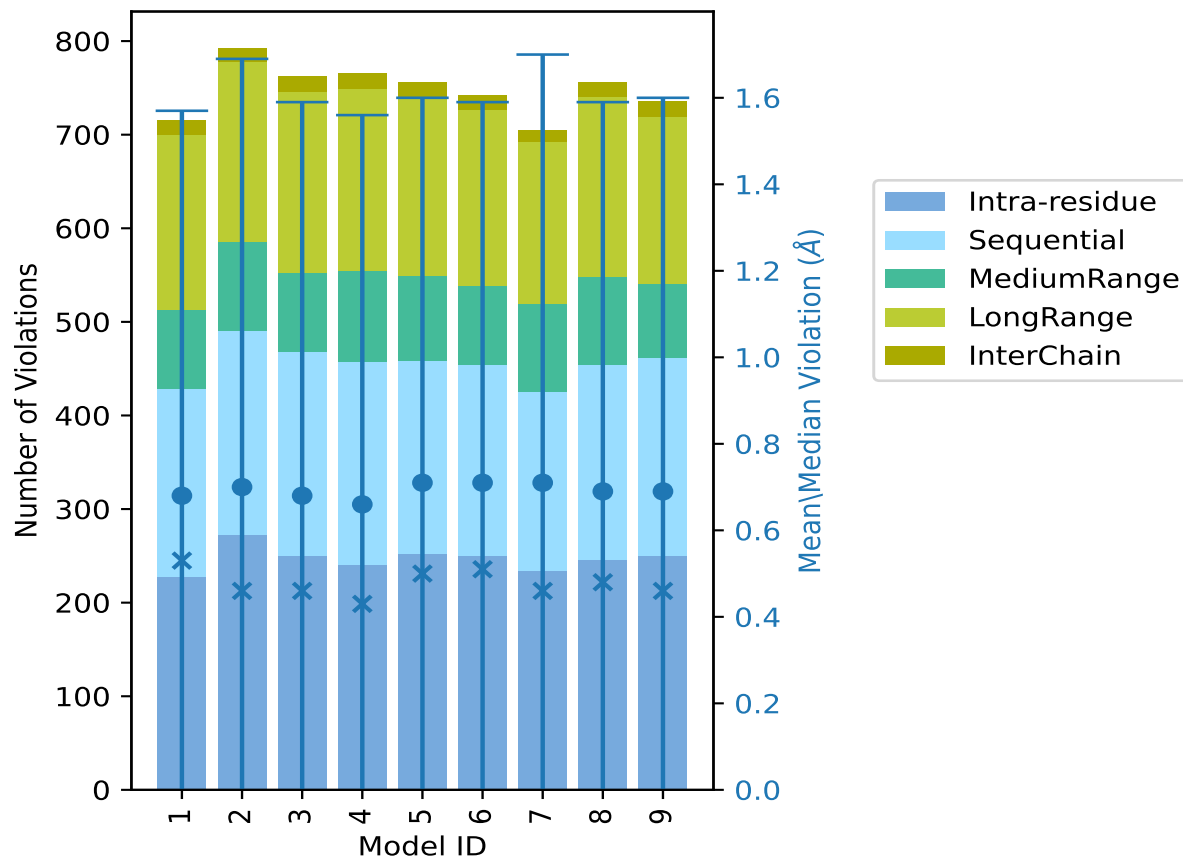
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 228                  | 200             | 85              | 187             | 16              | 716   | 0.68     | 18.39   | 0.89                | 0.53       |
| 2        | 273                  | 217             | 96              | 192             | 14              | 792   | 0.7      | 20.97   | 0.99                | 0.46       |
| 3        | 250                  | 218             | 84              | 194             | 17              | 763   | 0.68     | 18.73   | 0.91                | 0.46       |
| 4        | 241                  | 216             | 98              | 194             | 17              | 766   | 0.66     | 18.24   | 0.9                 | 0.43       |
| 5        | 252                  | 207             | 90              | 192             | 15              | 756   | 0.71     | 16.6    | 0.89                | 0.5        |
| 6        | 250                  | 204             | 84              | 188             | 16              | 742   | 0.71     | 16.85   | 0.88                | 0.51       |
| 7        | 234                  | 191             | 94              | 174             | 12              | 705   | 0.71     | 18.97   | 0.99                | 0.46       |
| 8        | 246                  | 208             | 94              | 193             | 15              | 756   | 0.69     | 18.48   | 0.9                 | 0.48       |
| 9        | 250                  | 211             | 80              | 178             | 17              | 736   | 0.69     | 17.84   | 0.91                | 0.46       |

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

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

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 534(IR:228, SQ:180, MR:52, LR:66, IC:8) 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>       | %    |
| 43                            | 42              | 14              | 37              | 7               | 143   | 1                        | 11.1 |
| 42                            | 31              | 22              | 48              | 4               | 147   | 2                        | 22.2 |
| 38                            | 32              | 7               | 39              | 0               | 116   | 3                        | 33.3 |
| 29                            | 27              | 11              | 20              | 4               | 91    | 4                        | 44.4 |
| 28                            | 22              | 20              | 32              | 0               | 102   | 5                        | 55.6 |
| 29                            | 16              | 18              | 36              | 1               | 100   | 6                        | 66.7 |

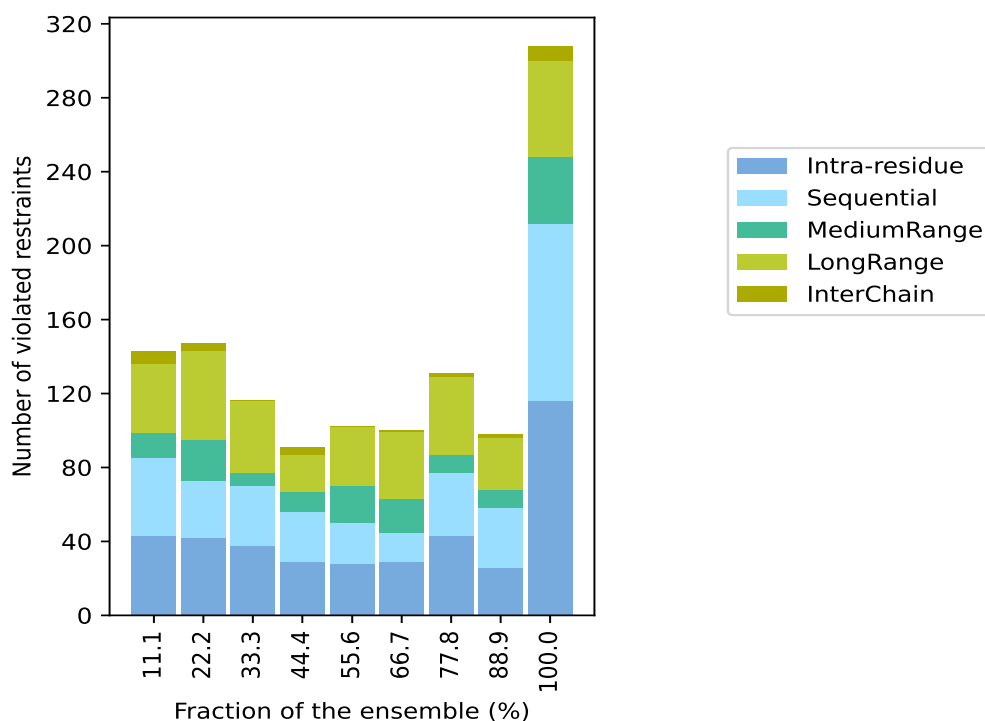
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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>       | %     |
| 43                            | 34              | 10              | 42              | 2               | 131   | 7                        | 77.8  |
| 26                            | 32              | 10              | 28              | 2               | 98    | 8                        | 88.9  |
| 116                           | 96              | 36              | 52              | 8               | 308   | 9                        | 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

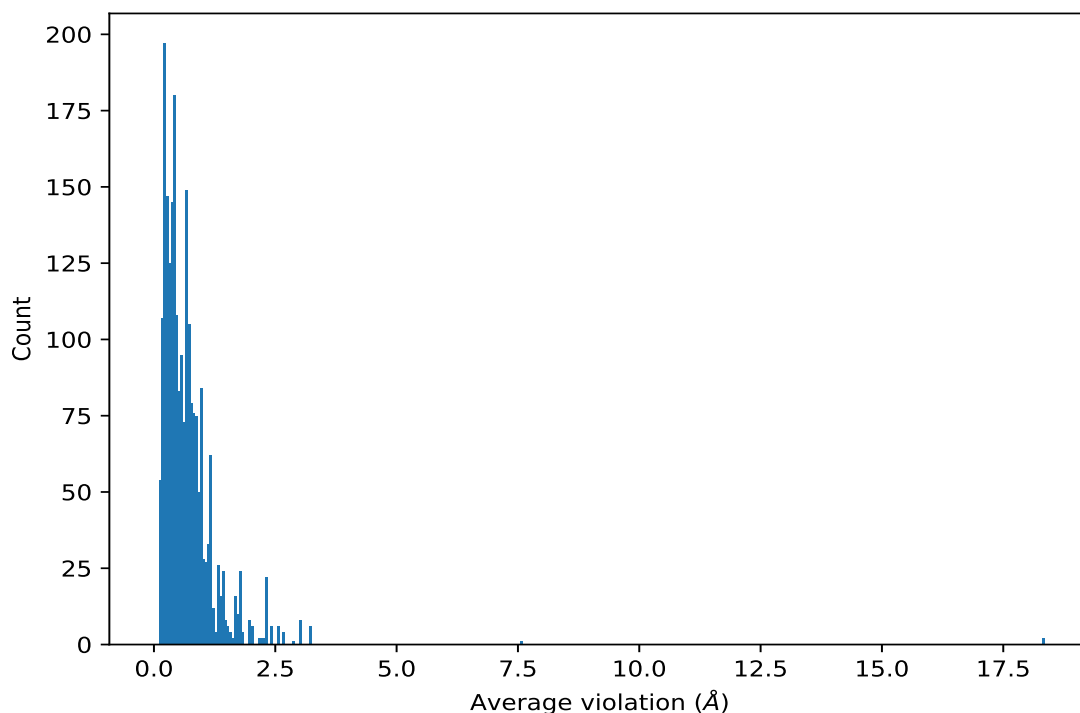
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1769) | 1:A:122:TYR:HD1  | 1:B:121:LYS:H    | 9                   | 18.34    | 1.2                 | 18.39      |
| (1,1769) | 1:A:122:TYR:HD2  | 1:B:121:LYS:H    | 9                   | 18.34    | 1.2                 | 18.39      |
| (1,1741) | 1:A:114:ILE:HA   | 1:B:116:ARG:HA   | 9                   | 7.56     | 0.54                | 7.47       |
| (1,1224) | 1:B:100:VAL:HG11 | 1:B:80:ASP:HA    | 9                   | 3.24     | 0.37                | 3.37       |
| (1,1224) | 1:B:100:VAL:HG12 | 1:B:80:ASP:HA    | 9                   | 3.24     | 0.37                | 3.37       |
| (1,1224) | 1:B:100:VAL:HG13 | 1:B:80:ASP:HA    | 9                   | 3.24     | 0.37                | 3.37       |
| (1,357)  | 1:A:100:VAL:HG11 | 1:A:80:ASP:HA    | 9                   | 3.24     | 0.37                | 3.37       |
| (1,357)  | 1:A:100:VAL:HG12 | 1:A:80:ASP:HA    | 9                   | 3.24     | 0.37                | 3.37       |
| (1,357)  | 1:A:100:VAL:HG13 | 1:A:80:ASP:HA    | 9                   | 3.24     | 0.37                | 3.37       |
| (1,436)  | 1:A:107:ARG:HB2  | 1:A:109:ASP:H    | 9                   | 3.03     | 0.23                | 3.09       |
| (1,1303) | 1:B:107:ARG:HB2  | 1:B:109:ASP:H    | 9                   | 3.03     | 0.23                | 3.09       |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG21 | 9                   | 3.02     | 0.68                | 3.16       |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG22 | 9                   | 3.02     | 0.68                | 3.16       |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG23 | 9                   | 3.02     | 0.68                | 3.16       |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG21 | 9                   | 3.01     | 0.68                | 3.15       |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG22 | 9                   | 3.01     | 0.68                | 3.15       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG23 | 9                   | 3.01     | 0.68                | 3.15       |
| (1,1754) | 1:A:118:PHE:HZ   | 1:B:116:ARG:HA   | 9                   | 2.86     | 1.1                 | 2.76       |
| (1,520)  | 1:A:115:SER:HA   | 1:A:104:HIS:HE1  | 9                   | 2.69     | 0.81                | 2.61       |
| (1,1387) | 1:B:115:SER:HA   | 1:B:104:HIS:HE1  | 9                   | 2.69     | 0.81                | 2.61       |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD1  | 9                   | 2.59     | 1.21                | 2.67       |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD2  | 9                   | 2.59     | 1.21                | 2.67       |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD1  | 9                   | 2.59     | 1.21                | 2.67       |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD2  | 9                   | 2.59     | 1.21                | 2.67       |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD1  | 9                   | 2.59     | 1.21                | 2.67       |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD2  | 9                   | 2.59     | 1.21                | 2.67       |
| (1,641)  | 1:A:124:ILE:HG21 | 1:A:148:PRO:HA   | 9                   | 2.42     | 0.73                | 2.39       |
| (1,641)  | 1:A:124:ILE:HG22 | 1:A:148:PRO:HA   | 9                   | 2.42     | 0.73                | 2.39       |
| (1,641)  | 1:A:124:ILE:HG23 | 1:A:148:PRO:HA   | 9                   | 2.42     | 0.73                | 2.39       |
| (1,1508) | 1:B:124:ILE:HG21 | 1:B:148:PRO:HA   | 9                   | 2.42     | 0.73                | 2.39       |
| (1,1508) | 1:B:124:ILE:HG22 | 1:B:148:PRO:HA   | 9                   | 2.42     | 0.73                | 2.39       |
| (1,1508) | 1:B:124:ILE:HG23 | 1:B:148:PRO:HA   | 9                   | 2.42     | 0.73                | 2.39       |
| (1,1761) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H    | 9                   | 2.31     | 1.1                 | 2.32       |
| (1,1761) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H    | 9                   | 2.31     | 1.1                 | 2.32       |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD1   | 9                   | 2.3      | 0.67                | 2.61       |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD2   | 9                   | 2.3      | 0.67                | 2.61       |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD1   | 9                   | 2.3      | 0.67                | 2.61       |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD2   | 9                   | 2.3      | 0.67                | 2.61       |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD1   | 9                   | 2.3      | 0.67                | 2.62       |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD2   | 9                   | 2.3      | 0.67                | 2.62       |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD1   | 9                   | 2.3      | 0.67                | 2.62       |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD2   | 9                   | 2.3      | 0.67                | 2.62       |
| (1,434)  | 1:A:107:ARG:HD3  | 1:A:109:ASP:H    | 9                   | 2.23     | 0.83                | 2.28       |
| (1,1301) | 1:B:107:ARG:HD3  | 1:B:109:ASP:H    | 9                   | 2.23     | 0.83                | 2.28       |
| (1,1322) | 1:B:111:HIS:HA   | 1:B:109:ASP:HA   | 9                   | 2.16     | 0.13                | 2.21       |
| (1,455)  | 1:A:111:HIS:HA   | 1:A:109:ASP:HA   | 9                   | 2.16     | 0.13                | 2.21       |
| (1,890)  | 1:B:70:LEU:HB2   | 1:B:74:ARG:H     | 9                   | 1.99     | 0.4                 | 2.07       |
| (1,23)   | 1:A:70:LEU:HB2   | 1:A:74:ARG:H     | 9                   | 1.99     | 0.4                 | 2.07       |
| (1,639)  | 1:A:124:ILE:HD11 | 1:A:128:VAL:H    | 9                   | 1.96     | 0.27                | 2.04       |
| (1,639)  | 1:A:124:ILE:HD12 | 1:A:128:VAL:H    | 9                   | 1.96     | 0.27                | 2.04       |
| (1,639)  | 1:A:124:ILE:HD13 | 1:A:128:VAL:H    | 9                   | 1.96     | 0.27                | 2.04       |
| (1,1506) | 1:B:124:ILE:HD11 | 1:B:128:VAL:H    | 9                   | 1.95     | 0.27                | 2.04       |
| (1,1506) | 1:B:124:ILE:HD12 | 1:B:128:VAL:H    | 9                   | 1.95     | 0.27                | 2.04       |
| (1,1506) | 1:B:124:ILE:HD13 | 1:B:128:VAL:H    | 9                   | 1.95     | 0.27                | 2.04       |
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG12 | 9                   | 1.84     | 0.52                | 1.56       |
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG13 | 9                   | 1.84     | 0.52                | 1.56       |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG12 | 9                   | 1.84     | 0.52                | 1.56       |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG13 | 9                   | 1.84     | 0.52                | 1.56       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,525)  | 1:A:115:SER:HB3  | 1:A:107:ARG:H    | 9                   | 1.77     | 0.3                 | 1.74       |
| (1,1392) | 1:B:115:SER:HB3  | 1:B:107:ARG:H    | 9                   | 1.77     | 0.3                 | 1.74       |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB2  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB3  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB2  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB3  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB2  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB3  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB2  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB3  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB2  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB3  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB2  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB3  | 9                   | 1.76     | 0.72                | 2.14       |
| (1,1319) | 1:B:109:ASP:H    | 1:B:114:ILE:HG13 | 9                   | 1.71     | 0.53                | 1.96       |
| (1,452)  | 1:A:109:ASP:H    | 1:A:114:ILE:HG13 | 9                   | 1.71     | 0.53                | 1.96       |
| (1,435)  | 1:A:107:ARG:HB3  | 1:A:109:ASP:H    | 9                   | 1.7      | 0.28                | 1.73       |
| (1,1302) | 1:B:107:ARG:HB3  | 1:B:109:ASP:H    | 9                   | 1.7      | 0.28                | 1.73       |
| (1,1760) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H    | 9                   | 1.68     | 1.1                 | 1.69       |
| (1,1760) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H    | 9                   | 1.68     | 1.1                 | 1.69       |
| (1,321)  | 1:A:97:VAL:H     | 1:A:93:VAL:HB    | 9                   | 1.62     | 1.21                | 1.06       |
| (1,1188) | 1:B:97:VAL:H     | 1:B:93:VAL:HB    | 9                   | 1.62     | 1.21                | 1.06       |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB2   | 9                   | 1.54     | 0.16                | 1.6        |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB3   | 9                   | 1.54     | 0.16                | 1.6        |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB2   | 9                   | 1.54     | 0.16                | 1.6        |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB3   | 9                   | 1.54     | 0.16                | 1.6        |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD11 | 9                   | 1.46     | 0.33                | 1.4        |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD12 | 9                   | 1.46     | 0.33                | 1.4        |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD13 | 9                   | 1.46     | 0.33                | 1.4        |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD11 | 9                   | 1.46     | 0.33                | 1.4        |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD12 | 9                   | 1.46     | 0.33                | 1.4        |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD13 | 9                   | 1.46     | 0.33                | 1.4        |
| (1,555)  | 1:A:118:PHE:HB2  | 1:A:117:GLU:H    | 9                   | 1.4      | 0.37                | 1.51       |
| (1,1422) | 1:B:118:PHE:HB2  | 1:B:117:GLU:H    | 9                   | 1.4      | 0.37                | 1.51       |
| (1,118)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB2  | 9                   | 1.36     | 0.4                 | 1.5        |
| (1,985)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB2  | 9                   | 1.36     | 0.4                 | 1.5        |
| (1,1348) | 1:B:113:PHE:HA   | 1:B:107:ARG:HB2  | 9                   | 1.31     | 0.34                | 1.38       |
| (1,481)  | 1:A:113:PHE:HA   | 1:A:107:ARG:HB2  | 9                   | 1.31     | 0.34                | 1.38       |
| (1,1121) | 1:B:89:LEU:HD11  | 1:B:91:VAL:HB    | 9                   | 1.3      | 0.86                | 1.2        |
| (1,1121) | 1:B:89:LEU:HD12  | 1:B:91:VAL:HB    | 9                   | 1.3      | 0.86                | 1.2        |
| (1,1121) | 1:B:89:LEU:HD13  | 1:B:91:VAL:HB    | 9                   | 1.3      | 0.86                | 1.2        |
| (1,254)  | 1:A:89:LEU:HD11  | 1:A:91:VAL:HB    | 9                   | 1.3      | 0.86                | 1.19       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,254)  | 1:A:89:LEU:HD12  | 1:A:91:VAL:HB    | 9                   | 1.3      | 0.86                | 1.19       |
| (1,254)  | 1:A:89:LEU:HD13  | 1:A:91:VAL:HB    | 9                   | 1.3      | 0.86                | 1.19       |
| (1,188)  | 1:A:83:HIS:H     | 1:A:141:GLY:HA2  | 9                   | 1.29     | 0.43                | 1.48       |
| (1,1055) | 1:B:83:HIS:H     | 1:B:141:GLY:HA2  | 9                   | 1.28     | 0.43                | 1.48       |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG12 | 9                   | 1.22     | 0.32                | 1.18       |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG13 | 9                   | 1.22     | 0.32                | 1.18       |
| (1,506)  | 1:A:114:ILE:HB   | 1:A:107:ARG:HD3  | 9                   | 1.22     | 0.77                | 1.04       |
| (1,1373) | 1:B:114:ILE:HB   | 1:B:107:ARG:HD3  | 9                   | 1.22     | 0.77                | 1.04       |
| (1,813)  | 1:A:145:VAL:HA   | 1:A:135:SER:H    | 9                   | 1.2      | 0.34                | 1.18       |
| (1,1680) | 1:B:145:VAL:HA   | 1:B:135:SER:H    | 9                   | 1.2      | 0.34                | 1.18       |
| (1,558)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HZ   | 9                   | 1.12     | 0.55                | 0.76       |
| (1,1425) | 1:B:118:PHE:HA   | 1:B:118:PHE:HZ   | 9                   | 1.11     | 0.54                | 0.76       |
| (1,1745) | 1:A:114:ILE:H    | 1:B:121:LYS:H    | 9                   | 1.11     | 0.28                | 1.07       |
| (1,652)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HA   | 9                   | 1.1      | 0.02                | 1.09       |
| (1,1519) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HA   | 9                   | 1.1      | 0.02                | 1.09       |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD2  | 9                   | 1.07     | 0.05                | 1.07       |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD3  | 9                   | 1.07     | 0.05                | 1.07       |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD2  | 9                   | 1.07     | 0.06                | 1.07       |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD3  | 9                   | 1.07     | 0.06                | 1.07       |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG21 | 9                   | 1.05     | 0.2                 | 1.07       |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG22 | 9                   | 1.05     | 0.2                 | 1.07       |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG23 | 9                   | 1.05     | 0.2                 | 1.07       |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG21 | 9                   | 1.05     | 0.21                | 1.07       |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG22 | 9                   | 1.05     | 0.21                | 1.07       |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG23 | 9                   | 1.05     | 0.21                | 1.07       |
| (1,1253) | 1:B:102:GLY:HA2  | 1:B:102:GLY:HA3  | 9                   | 1.0      | 0.01                | 1.0        |
| (1,386)  | 1:A:102:GLY:HA2  | 1:A:102:GLY:HA3  | 9                   | 1.0      | 0.01                | 1.0        |
| (1,1591) | 1:B:133:ILE:HD11 | 1:B:134:THR:H    | 9                   | 0.99     | 0.27                | 1.11       |
| (1,1591) | 1:B:133:ILE:HD12 | 1:B:134:THR:H    | 9                   | 0.99     | 0.27                | 1.11       |
| (1,1591) | 1:B:133:ILE:HD13 | 1:B:134:THR:H    | 9                   | 0.99     | 0.27                | 1.11       |
| (1,724)  | 1:A:133:ILE:HD11 | 1:A:134:THR:H    | 9                   | 0.99     | 0.26                | 1.11       |
| (1,724)  | 1:A:133:ILE:HD12 | 1:A:134:THR:H    | 9                   | 0.99     | 0.26                | 1.11       |
| (1,724)  | 1:A:133:ILE:HD13 | 1:A:134:THR:H    | 9                   | 0.99     | 0.26                | 1.11       |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB2  | 9                   | 0.97     | 0.28                | 0.92       |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB3  | 9                   | 0.97     | 0.28                | 0.92       |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB2  | 9                   | 0.96     | 0.28                | 0.91       |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB3  | 9                   | 0.96     | 0.28                | 0.91       |
| (1,490)  | 1:A:113:PHE:HD1  | 1:A:113:PHE:HB2  | 9                   | 0.94     | 0.04                | 0.94       |
| (1,490)  | 1:A:113:PHE:HD2  | 1:A:113:PHE:HB2  | 9                   | 0.94     | 0.04                | 0.94       |
| (1,1357) | 1:B:113:PHE:HD1  | 1:B:113:PHE:HB2  | 9                   | 0.94     | 0.04                | 0.94       |
| (1,1357) | 1:B:113:PHE:HD2  | 1:B:113:PHE:HB2  | 9                   | 0.94     | 0.04                | 0.94       |
| (1,96)   | 1:A:77:VAL:HG21  | 1:A:77:VAL:HB    | 9                   | 0.93     | 0.01                | 0.93       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,96)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:HB   | 9                   | 0.93     | 0.01                | 0.93       |
| (1,96)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:HB   | 9                   | 0.93     | 0.01                | 0.93       |
| (1,963)  | 1:B:77:VAL:HG21 | 1:B:77:VAL:HB   | 9                   | 0.93     | 0.01                | 0.93       |
| (1,963)  | 1:B:77:VAL:HG22 | 1:B:77:VAL:HB   | 9                   | 0.93     | 0.01                | 0.93       |
| (1,963)  | 1:B:77:VAL:HG23 | 1:B:77:VAL:HB   | 9                   | 0.93     | 0.01                | 0.93       |
| (1,744)  | 1:A:135:SER:HB3 | 1:A:146:ASP:H   | 9                   | 0.92     | 0.5                 | 0.69       |
| (1,1611) | 1:B:135:SER:HB3 | 1:B:146:ASP:H   | 9                   | 0.92     | 0.5                 | 0.69       |
| (1,1090) | 1:B:87:GLU:H    | 1:B:88:GLU:HB2  | 9                   | 0.88     | 0.24                | 0.85       |
| (1,1090) | 1:B:87:GLU:H    | 1:B:88:GLU:HB3  | 9                   | 0.88     | 0.24                | 0.85       |
| (1,223)  | 1:A:87:GLU:H    | 1:A:88:GLU:HB2  | 9                   | 0.88     | 0.23                | 0.85       |
| (1,223)  | 1:A:87:GLU:H    | 1:A:88:GLU:HB3  | 9                   | 0.88     | 0.23                | 0.85       |
| (1,651)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HA  | 9                   | 0.87     | 0.04                | 0.88       |
| (1,1518) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HA  | 9                   | 0.87     | 0.04                | 0.87       |
| (1,1155) | 1:B:93:VAL:HA   | 1:B:99:GLU:H    | 9                   | 0.87     | 0.32                | 1.02       |
| (1,288)  | 1:A:93:VAL:HA   | 1:A:99:GLU:H    | 9                   | 0.87     | 0.32                | 1.02       |
| (1,846)  | 1:A:147:GLY:HA2 | 1:A:147:GLY:HA3 | 9                   | 0.87     | 0.01                | 0.87       |
| (1,1713) | 1:B:147:GLY:HA2 | 1:B:147:GLY:HA3 | 9                   | 0.87     | 0.02                | 0.87       |
| (1,433)  | 1:A:107:ARG:HB3 | 1:A:108:GLN:H   | 9                   | 0.85     | 0.02                | 0.85       |
| (1,1300) | 1:B:107:ARG:HB3 | 1:B:108:GLN:H   | 9                   | 0.85     | 0.02                | 0.85       |
| (1,841)  | 1:A:147:GLY:HA2 | 1:A:132:THR:HA  | 9                   | 0.83     | 0.21                | 0.91       |
| (1,1708) | 1:B:147:GLY:HA2 | 1:B:132:THR:HA  | 9                   | 0.83     | 0.21                | 0.91       |
| (1,1464) | 1:B:122:TYR:HB2 | 1:B:122:TYR:H   | 9                   | 0.82     | 0.27                | 0.94       |
| (1,1464) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H   | 9                   | 0.82     | 0.27                | 0.94       |
| (1,1465) | 1:B:122:TYR:HB2 | 1:B:122:TYR:H   | 9                   | 0.82     | 0.27                | 0.94       |
| (1,1465) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H   | 9                   | 0.82     | 0.27                | 0.94       |
| (1,597)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:H   | 9                   | 0.82     | 0.27                | 0.94       |
| (1,597)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:H   | 9                   | 0.82     | 0.27                | 0.94       |
| (1,598)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:H   | 9                   | 0.82     | 0.27                | 0.94       |
| (1,598)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:H   | 9                   | 0.82     | 0.27                | 0.94       |
| (1,338)  | 1:A:98:ILE:HG21 | 1:A:98:ILE:HB   | 9                   | 0.81     | 0.01                | 0.81       |
| (1,338)  | 1:A:98:ILE:HG22 | 1:A:98:ILE:HB   | 9                   | 0.81     | 0.01                | 0.81       |
| (1,338)  | 1:A:98:ILE:HG23 | 1:A:98:ILE:HB   | 9                   | 0.81     | 0.01                | 0.81       |
| (1,1205) | 1:B:98:ILE:HG21 | 1:B:98:ILE:HB   | 9                   | 0.81     | 0.01                | 0.81       |
| (1,1205) | 1:B:98:ILE:HG22 | 1:B:98:ILE:HB   | 9                   | 0.81     | 0.01                | 0.81       |
| (1,1205) | 1:B:98:ILE:HG23 | 1:B:98:ILE:HB   | 9                   | 0.81     | 0.01                | 0.81       |
| (1,1380) | 1:B:114:ILE:HA  | 1:B:114:ILE:HB  | 9                   | 0.8      | 0.19                | 0.86       |
| (1,513)  | 1:A:114:ILE:HA  | 1:A:114:ILE:HB  | 9                   | 0.8      | 0.19                | 0.86       |
| (1,381)  | 1:A:101:HIS:HA  | 1:A:102:GLY:H   | 9                   | 0.79     | 0.13                | 0.77       |
| (1,1248) | 1:B:101:HIS:HA  | 1:B:102:GLY:H   | 9                   | 0.79     | 0.13                | 0.77       |
| (1,958)  | 1:B:77:VAL:HG11 | 1:B:77:VAL:HB   | 9                   | 0.78     | 0.01                | 0.78       |
| (1,958)  | 1:B:77:VAL:HG12 | 1:B:77:VAL:HB   | 9                   | 0.78     | 0.01                | 0.78       |
| (1,958)  | 1:B:77:VAL:HG13 | 1:B:77:VAL:HB   | 9                   | 0.78     | 0.01                | 0.78       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,703)  | 1:A:132:THR:HA   | 1:A:133:ILE:HA   | 9                   | 0.78     | 0.04                | 0.79       |
| (1,91)   | 1:A:77:VAL:HG11  | 1:A:77:VAL:HB    | 9                   | 0.78     | 0.01                | 0.78       |
| (1,91)   | 1:A:77:VAL:HG12  | 1:A:77:VAL:HB    | 9                   | 0.78     | 0.01                | 0.78       |
| (1,91)   | 1:A:77:VAL:HG13  | 1:A:77:VAL:HB    | 9                   | 0.78     | 0.01                | 0.78       |
| (1,1570) | 1:B:132:THR:HA   | 1:B:133:ILE:HA   | 9                   | 0.78     | 0.04                | 0.78       |
| (1,758)  | 1:A:138:SER:HA   | 1:A:141:GLY:H    | 9                   | 0.77     | 0.12                | 0.74       |
| (1,1625) | 1:B:138:SER:HA   | 1:B:141:GLY:H    | 9                   | 0.77     | 0.12                | 0.74       |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD2   | 9                   | 0.76     | 0.22                | 0.66       |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD3   | 9                   | 0.76     | 0.22                | 0.66       |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD2   | 9                   | 0.75     | 0.22                | 0.66       |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD3   | 9                   | 0.75     | 0.22                | 0.66       |
| (1,497)  | 1:A:113:PHE:HD1  | 1:A:113:PHE:H    | 9                   | 0.75     | 0.36                | 0.78       |
| (1,497)  | 1:A:113:PHE:HD2  | 1:A:113:PHE:H    | 9                   | 0.75     | 0.36                | 0.78       |
| (1,1364) | 1:B:113:PHE:HD1  | 1:B:113:PHE:H    | 9                   | 0.75     | 0.36                | 0.78       |
| (1,1364) | 1:B:113:PHE:HD2  | 1:B:113:PHE:H    | 9                   | 0.75     | 0.36                | 0.78       |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD11 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD12 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD13 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD11 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD12 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD13 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD11 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD12 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD13 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD11 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD12 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD13 | 9                   | 0.75     | 0.01                | 0.74       |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG2   | 9                   | 0.74     | 0.41                | 0.75       |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG3   | 9                   | 0.74     | 0.41                | 0.75       |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG2   | 9                   | 0.74     | 0.41                | 0.75       |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG3   | 9                   | 0.74     | 0.41                | 0.75       |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD11 | 9                   | 0.74     | 0.05                | 0.74       |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD12 | 9                   | 0.74     | 0.05                | 0.74       |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD13 | 9                   | 0.74     | 0.05                | 0.74       |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD11 | 9                   | 0.74     | 0.05                | 0.74       |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD12 | 9                   | 0.74     | 0.05                | 0.74       |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD13 | 9                   | 0.74     | 0.05                | 0.74       |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD11 | 9                   | 0.74     | 0.05                | 0.74       |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD12 | 9                   | 0.74     | 0.05                | 0.74       |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD13 | 9                   | 0.74     | 0.05                | 0.74       |
| (1,681)  | 1:A:128:VAL:H    | 1:A:150:LYS:HD2  | 9                   | 0.74     | 0.87                | 0.18       |
| (1,681)  | 1:A:128:VAL:H    | 1:A:150:LYS:HD3  | 9                   | 0.74     | 0.87                | 0.18       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD2  | 9                   | 0.74     | 0.87                | 0.18       |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD3  | 9                   | 0.74     | 0.87                | 0.18       |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD11 | 9                   | 0.74     | 0.05                | 0.73       |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD12 | 9                   | 0.74     | 0.05                | 0.73       |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD13 | 9                   | 0.74     | 0.05                | 0.73       |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD11 | 9                   | 0.74     | 0.05                | 0.73       |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD12 | 9                   | 0.74     | 0.05                | 0.73       |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD13 | 9                   | 0.74     | 0.05                | 0.73       |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD11 | 9                   | 0.74     | 0.05                | 0.73       |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD12 | 9                   | 0.74     | 0.05                | 0.73       |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD13 | 9                   | 0.74     | 0.05                | 0.73       |
| (1,1710) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HB   | 9                   | 0.73     | 0.24                | 0.8        |
| (1,843)  | 1:A:147:GLY:HA2  | 1:A:133:ILE:HB   | 9                   | 0.73     | 0.24                | 0.8        |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB2  | 9                   | 0.72     | 0.1                 | 0.75       |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB3  | 9                   | 0.72     | 0.1                 | 0.75       |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB2  | 9                   | 0.72     | 0.1                 | 0.75       |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB3  | 9                   | 0.72     | 0.1                 | 0.75       |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD11 | 9                   | 0.72     | 0.04                | 0.72       |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD12 | 9                   | 0.72     | 0.04                | 0.72       |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD13 | 9                   | 0.72     | 0.04                | 0.72       |
| (1,255)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2  | 9                   | 0.71     | 0.09                | 0.71       |
| (1,256)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2  | 9                   | 0.71     | 0.09                | 0.71       |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD11 | 9                   | 0.71     | 0.04                | 0.71       |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD12 | 9                   | 0.71     | 0.04                | 0.71       |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD13 | 9                   | 0.71     | 0.04                | 0.71       |
| (1,631)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.71       |
| (1,631)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.71       |
| (1,631)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.71       |
| (1,632)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.71       |
| (1,632)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.71       |
| (1,632)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.71       |
| (1,1122) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2  | 9                   | 0.71     | 0.08                | 0.71       |
| (1,1123) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2  | 9                   | 0.71     | 0.08                | 0.71       |
| (1,1498) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.7        |
| (1,1498) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.7        |
| (1,1498) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.7        |
| (1,1499) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.7        |
| (1,1499) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.7        |
| (1,1499) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 9                   | 0.71     | 0.04                | 0.7        |
| (1,956)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 9                   | 0.7      | 0.05                | 0.73       |
| (1,956)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 9                   | 0.7      | 0.05                | 0.73       |
| (1,956)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 9                   | 0.7      | 0.05                | 0.73       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 9                   | 0.7      | 0.05                | 0.73       |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 9                   | 0.7      | 0.05                | 0.73       |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 9                   | 0.7      | 0.05                | 0.73       |
| (1,89)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 9                   | 0.69     | 0.05                | 0.73       |
| (1,89)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 9                   | 0.69     | 0.05                | 0.73       |
| (1,89)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 9                   | 0.69     | 0.05                | 0.73       |
| (1,95)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 9                   | 0.69     | 0.05                | 0.73       |
| (1,95)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 9                   | 0.69     | 0.05                | 0.73       |
| (1,95)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 9                   | 0.69     | 0.05                | 0.73       |
| (1,149)  | 1:A:80:ASP:HA    | 1:A:81:VAL:H     | 9                   | 0.69     | 0.01                | 0.7        |
| (1,1016) | 1:B:80:ASP:HA    | 1:B:81:VAL:H     | 9                   | 0.69     | 0.02                | 0.7        |
| (1,475)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 9                   | 0.68     | 0.01                | 0.68       |
| (1,476)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 9                   | 0.68     | 0.01                | 0.68       |
| (1,1342) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 9                   | 0.68     | 0.01                | 0.68       |
| (1,1343) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 9                   | 0.68     | 0.01                | 0.68       |
| (1,105)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HG    | 9                   | 0.67     | 0.76                | 0.44       |
| (1,105)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HG    | 9                   | 0.67     | 0.76                | 0.44       |
| (1,105)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HG    | 9                   | 0.67     | 0.76                | 0.44       |
| (1,972)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HG    | 9                   | 0.67     | 0.76                | 0.44       |
| (1,972)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HG    | 9                   | 0.67     | 0.76                | 0.44       |
| (1,972)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HG    | 9                   | 0.67     | 0.76                | 0.44       |
| (1,1581) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HA   | 9                   | 0.66     | 0.13                | 0.67       |
| (1,1581) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HA   | 9                   | 0.66     | 0.13                | 0.67       |
| (1,1581) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HA   | 9                   | 0.66     | 0.13                | 0.67       |
| (1,714)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HA   | 9                   | 0.66     | 0.13                | 0.67       |
| (1,714)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HA   | 9                   | 0.66     | 0.13                | 0.67       |
| (1,714)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HA   | 9                   | 0.66     | 0.13                | 0.67       |
| (1,458)  | 1:A:111:HIS:H    | 1:A:110:GLU:H    | 9                   | 0.66     | 0.28                | 0.76       |
| (1,459)  | 1:A:111:HIS:H    | 1:A:110:GLU:H    | 9                   | 0.66     | 0.28                | 0.76       |
| (1,1325) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 9                   | 0.66     | 0.28                | 0.76       |
| (1,1326) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 9                   | 0.66     | 0.28                | 0.76       |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG21 | 9                   | 0.64     | 0.11                | 0.65       |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG22 | 9                   | 0.64     | 0.11                | 0.65       |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG23 | 9                   | 0.64     | 0.11                | 0.65       |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG21 | 9                   | 0.64     | 0.11                | 0.65       |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG22 | 9                   | 0.64     | 0.11                | 0.65       |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG23 | 9                   | 0.64     | 0.11                | 0.65       |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG21 | 9                   | 0.64     | 0.11                | 0.65       |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG22 | 9                   | 0.64     | 0.11                | 0.65       |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG23 | 9                   | 0.64     | 0.11                | 0.65       |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG21 | 9                   | 0.64     | 0.11                | 0.65       |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG22 | 9                   | 0.64     | 0.11                | 0.65       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG23 | 9                   | 0.64     | 0.11                | 0.65       |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG21 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG22 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG23 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG21 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG22 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG23 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG21 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG22 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG23 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG21 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG22 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG23 | 9                   | 0.64     | 0.03                | 0.64       |
| (1,548)  | 1:A:117:GLU:HA   | 1:A:118:PHE:H    | 9                   | 0.63     | 0.09                | 0.68       |
| (1,1415) | 1:B:117:GLU:HA   | 1:B:118:PHE:H    | 9                   | 0.63     | 0.09                | 0.68       |
| (1,857)  | 1:A:150:LYS:H    | 1:A:150:LYS:HD2  | 9                   | 0.62     | 0.28                | 0.58       |
| (1,857)  | 1:A:150:LYS:H    | 1:A:150:LYS:HD3  | 9                   | 0.62     | 0.28                | 0.58       |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD2  | 9                   | 0.62     | 0.28                | 0.58       |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD3  | 9                   | 0.62     | 0.28                | 0.58       |
| (1,443)  | 1:A:108:GLN:HA   | 1:A:109:ASP:H    | 9                   | 0.6      | 0.02                | 0.59       |
| (1,1310) | 1:B:108:GLN:HA   | 1:B:109:ASP:H    | 9                   | 0.6      | 0.02                | 0.59       |
| (1,199)  | 1:A:84:PHE:HB2   | 1:A:85:SER:H     | 9                   | 0.59     | 0.3                 | 0.45       |
| (1,199)  | 1:A:84:PHE:HB3   | 1:A:85:SER:H     | 9                   | 0.59     | 0.3                 | 0.45       |
| (1,584)  | 1:A:121:LYS:HA   | 1:A:120:ARG:HB2  | 9                   | 0.59     | 0.14                | 0.57       |
| (1,584)  | 1:A:121:LYS:HA   | 1:A:120:ARG:HB3  | 9                   | 0.59     | 0.14                | 0.57       |
| (1,1066) | 1:B:84:PHE:HB2   | 1:B:85:SER:H     | 9                   | 0.59     | 0.3                 | 0.45       |
| (1,1066) | 1:B:84:PHE:HB3   | 1:B:85:SER:H     | 9                   | 0.59     | 0.3                 | 0.45       |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB2  | 9                   | 0.59     | 0.14                | 0.57       |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB3  | 9                   | 0.59     | 0.14                | 0.57       |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD2  | 9                   | 0.58     | 0.14                | 0.68       |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD3  | 9                   | 0.58     | 0.14                | 0.68       |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD2  | 9                   | 0.58     | 0.14                | 0.68       |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD3  | 9                   | 0.58     | 0.14                | 0.68       |
| (1,1407) | 1:B:116:ARG:HA   | 1:B:117:GLU:H    | 9                   | 0.58     | 0.08                | 0.62       |
| (1,540)  | 1:A:116:ARG:HA   | 1:A:117:GLU:H    | 9                   | 0.58     | 0.09                | 0.62       |
| (1,583)  | 1:A:121:LYS:HA   | 1:A:99:GLU:HA    | 9                   | 0.57     | 0.15                | 0.65       |
| (1,1450) | 1:B:121:LYS:HA   | 1:B:99:GLU:HA    | 9                   | 0.57     | 0.15                | 0.65       |
| (1,840)  | 1:A:146:ASP:HA   | 1:A:147:GLY:H    | 9                   | 0.57     | 0.07                | 0.59       |
| (1,1707) | 1:B:146:ASP:HA   | 1:B:147:GLY:H    | 9                   | 0.57     | 0.07                | 0.59       |
| (1,1176) | 1:B:96:ASP:H     | 1:B:95:GLY:H     | 9                   | 0.56     | 0.07                | 0.57       |
| (1,309)  | 1:A:96:ASP:H     | 1:A:95:GLY:H     | 9                   | 0.56     | 0.07                | 0.57       |
| (1,566)  | 1:A:118:PHE:HA   | 1:A:119:HIS:H    | 9                   | 0.56     | 0.1                 | 0.52       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1433) | 1:B:118:PHE:HA   | 1:B:119:HIS:H   | 9                   | 0.56     | 0.1                 | 0.52       |
| (1,1175) | 1:B:96:ASP:H     | 1:B:95:GLY:H    | 9                   | 0.55     | 0.07                | 0.56       |
| (1,308)  | 1:A:96:ASP:H     | 1:A:95:GLY:H    | 9                   | 0.55     | 0.07                | 0.56       |
| (1,155)  | 1:A:81:VAL:HG11  | 1:A:81:VAL:HA   | 9                   | 0.55     | 0.08                | 0.6        |
| (1,155)  | 1:A:81:VAL:HG12  | 1:A:81:VAL:HA   | 9                   | 0.55     | 0.08                | 0.6        |
| (1,155)  | 1:A:81:VAL:HG13  | 1:A:81:VAL:HA   | 9                   | 0.55     | 0.08                | 0.6        |
| (1,1022) | 1:B:81:VAL:HG11  | 1:B:81:VAL:HA   | 9                   | 0.55     | 0.08                | 0.6        |
| (1,1022) | 1:B:81:VAL:HG12  | 1:B:81:VAL:HA   | 9                   | 0.55     | 0.08                | 0.6        |
| (1,1022) | 1:B:81:VAL:HG13  | 1:B:81:VAL:HA   | 9                   | 0.55     | 0.08                | 0.6        |
| (1,1666) | 1:B:144:THR:HG21 | 1:B:144:THR:HA  | 9                   | 0.54     | 0.02                | 0.54       |
| (1,1666) | 1:B:144:THR:HG22 | 1:B:144:THR:HA  | 9                   | 0.54     | 0.02                | 0.54       |
| (1,1666) | 1:B:144:THR:HG23 | 1:B:144:THR:HA  | 9                   | 0.54     | 0.02                | 0.54       |
| (1,301)  | 1:A:95:GLY:H     | 1:A:94:LEU:HG   | 9                   | 0.54     | 0.32                | 0.43       |
| (1,1168) | 1:B:95:GLY:H     | 1:B:94:LEU:HG   | 9                   | 0.54     | 0.32                | 0.42       |
| (1,799)  | 1:A:144:THR:HG21 | 1:A:144:THR:HA  | 9                   | 0.54     | 0.01                | 0.54       |
| (1,799)  | 1:A:144:THR:HG22 | 1:A:144:THR:HA  | 9                   | 0.54     | 0.01                | 0.54       |
| (1,799)  | 1:A:144:THR:HG23 | 1:A:144:THR:HA  | 9                   | 0.54     | 0.01                | 0.54       |
| (1,848)  | 1:A:147:GLY:HA3  | 1:A:147:GLY:H   | 9                   | 0.53     | 0.11                | 0.54       |
| (1,1715) | 1:B:147:GLY:HA3  | 1:B:147:GLY:H   | 9                   | 0.53     | 0.11                | 0.54       |
| (1,437)  | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD1 | 9                   | 0.52     | 0.19                | 0.6        |
| (1,437)  | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD2 | 9                   | 0.52     | 0.19                | 0.6        |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD1 | 9                   | 0.52     | 0.19                | 0.6        |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD2 | 9                   | 0.52     | 0.19                | 0.6        |
| (1,1138) | 1:B:91:VAL:HB    | 1:B:92:LYS:H    | 9                   | 0.52     | 0.08                | 0.53       |
| (1,271)  | 1:A:91:VAL:HB    | 1:A:92:LYS:H    | 9                   | 0.52     | 0.08                | 0.53       |
| (1,717)  | 1:A:133:ILE:HG21 | 1:A:132:THR:H   | 9                   | 0.51     | 0.17                | 0.58       |
| (1,717)  | 1:A:133:ILE:HG22 | 1:A:132:THR:H   | 9                   | 0.51     | 0.17                | 0.58       |
| (1,717)  | 1:A:133:ILE:HG23 | 1:A:132:THR:H   | 9                   | 0.51     | 0.17                | 0.58       |
| (1,1584) | 1:B:133:ILE:HG21 | 1:B:132:THR:H   | 9                   | 0.51     | 0.17                | 0.58       |
| (1,1584) | 1:B:133:ILE:HG22 | 1:B:132:THR:H   | 9                   | 0.51     | 0.17                | 0.58       |
| (1,1584) | 1:B:133:ILE:HG23 | 1:B:132:THR:H   | 9                   | 0.51     | 0.17                | 0.58       |
| (1,974)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HG   | 9                   | 0.5      | 0.13                | 0.5        |
| (1,974)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HG   | 9                   | 0.5      | 0.13                | 0.5        |
| (1,974)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HG   | 9                   | 0.5      | 0.13                | 0.5        |
| (1,107)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:HG   | 9                   | 0.5      | 0.13                | 0.5        |
| (1,107)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:HG   | 9                   | 0.5      | 0.13                | 0.5        |
| (1,107)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:HG   | 9                   | 0.5      | 0.13                | 0.5        |
| (1,323)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HB2  | 9                   | 0.49     | 0.08                | 0.49       |
| (1,323)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HB3  | 9                   | 0.49     | 0.08                | 0.49       |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB2  | 9                   | 0.49     | 0.08                | 0.49       |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB3  | 9                   | 0.49     | 0.08                | 0.49       |
| (1,1397) | 1:B:115:SER:HB2  | 1:B:115:SER:HB3 | 9                   | 0.49     | 0.01                | 0.49       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,530)  | 1:A:115:SER:HB2  | 1:A:115:SER:HB3  | 9                   | 0.49     | 0.01                | 0.49       |
| (1,633)  | 1:A:124:ILE:HA   | 1:A:124:ILE:H    | 9                   | 0.48     | 0.05                | 0.47       |
| (1,1500) | 1:B:124:ILE:HA   | 1:B:124:ILE:H    | 9                   | 0.48     | 0.05                | 0.47       |
| (1,354)  | 1:A:99:GLU:HA    | 1:A:100:VAL:H    | 9                   | 0.48     | 0.08                | 0.49       |
| (1,1221) | 1:B:99:GLU:HA    | 1:B:100:VAL:H    | 9                   | 0.48     | 0.08                | 0.49       |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD11  | 9                   | 0.47     | 0.34                | 0.38       |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD12  | 9                   | 0.47     | 0.34                | 0.38       |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD13  | 9                   | 0.47     | 0.34                | 0.38       |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD21  | 9                   | 0.47     | 0.34                | 0.38       |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD22  | 9                   | 0.47     | 0.34                | 0.38       |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD23  | 9                   | 0.47     | 0.34                | 0.38       |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD11  | 9                   | 0.47     | 0.34                | 0.37       |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD12  | 9                   | 0.47     | 0.34                | 0.37       |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD13  | 9                   | 0.47     | 0.34                | 0.37       |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD21  | 9                   | 0.47     | 0.34                | 0.37       |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD22  | 9                   | 0.47     | 0.34                | 0.37       |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD23  | 9                   | 0.47     | 0.34                | 0.37       |
| (1,562)  | 1:A:118:PHE:HA   | 1:A:118:PHE:H    | 9                   | 0.47     | 0.03                | 0.47       |
| (1,1429) | 1:B:118:PHE:HA   | 1:B:118:PHE:H    | 9                   | 0.47     | 0.03                | 0.46       |
| (1,586)  | 1:A:121:LYS:HA   | 1:A:122:TYR:H    | 9                   | 0.46     | 0.08                | 0.45       |
| (1,1453) | 1:B:121:LYS:HA   | 1:B:122:TYR:H    | 9                   | 0.46     | 0.08                | 0.45       |
| (1,1501) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 9                   | 0.46     | 0.08                | 0.47       |
| (1,1501) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 9                   | 0.46     | 0.08                | 0.47       |
| (1,1501) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H    | 9                   | 0.46     | 0.08                | 0.47       |
| (1,1502) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 9                   | 0.46     | 0.08                | 0.47       |
| (1,1502) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 9                   | 0.46     | 0.08                | 0.47       |
| (1,1502) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H    | 9                   | 0.46     | 0.08                | 0.47       |
| (1,634)  | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 9                   | 0.45     | 0.08                | 0.46       |
| (1,634)  | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 9                   | 0.45     | 0.08                | 0.46       |
| (1,634)  | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 9                   | 0.45     | 0.08                | 0.46       |
| (1,635)  | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 9                   | 0.45     | 0.08                | 0.46       |
| (1,635)  | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 9                   | 0.45     | 0.08                | 0.46       |
| (1,635)  | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 9                   | 0.45     | 0.08                | 0.46       |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG11 | 9                   | 0.45     | 0.16                | 0.55       |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG12 | 9                   | 0.45     | 0.16                | 0.55       |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG13 | 9                   | 0.45     | 0.16                | 0.55       |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG21 | 9                   | 0.45     | 0.16                | 0.55       |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG22 | 9                   | 0.45     | 0.16                | 0.55       |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG23 | 9                   | 0.45     | 0.16                | 0.55       |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG11 | 9                   | 0.44     | 0.16                | 0.54       |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG12 | 9                   | 0.44     | 0.16                | 0.54       |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG13 | 9                   | 0.44     | 0.16                | 0.54       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG21 | 9                   | 0.44     | 0.16                | 0.54       |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG22 | 9                   | 0.44     | 0.16                | 0.54       |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG23 | 9                   | 0.44     | 0.16                | 0.54       |
| (1,329)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA   | 9                   | 0.44     | 0.15                | 0.47       |
| (1,330)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA   | 9                   | 0.44     | 0.15                | 0.47       |
| (1,1196) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA   | 9                   | 0.44     | 0.15                | 0.47       |
| (1,1197) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA   | 9                   | 0.44     | 0.15                | 0.47       |
| (1,791)  | 1:A:143:LEU:HA   | 1:A:144:THR:H    | 9                   | 0.43     | 0.01                | 0.43       |
| (1,1658) | 1:B:143:LEU:HA   | 1:B:144:THR:H    | 9                   | 0.43     | 0.01                | 0.43       |
| (1,629)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG12 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,629)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG13 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,629)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG12 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,629)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG13 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,629)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG12 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,629)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG13 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG12 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG13 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG12 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG13 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG12 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG13 | 9                   | 0.42     | 0.02                | 0.42       |
| (1,738)  | 1:A:135:SER:HA   | 1:A:145:VAL:HG21 | 9                   | 0.42     | 0.19                | 0.43       |
| (1,738)  | 1:A:135:SER:HA   | 1:A:145:VAL:HG22 | 9                   | 0.42     | 0.19                | 0.43       |
| (1,738)  | 1:A:135:SER:HA   | 1:A:145:VAL:HG23 | 9                   | 0.42     | 0.19                | 0.43       |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG21 | 9                   | 0.42     | 0.19                | 0.44       |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG22 | 9                   | 0.42     | 0.19                | 0.44       |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG23 | 9                   | 0.42     | 0.19                | 0.44       |
| (1,1457) | 1:B:122:TYR:HA   | 1:B:98:ILE:H     | 9                   | 0.41     | 0.17                | 0.45       |
| (1,590)  | 1:A:122:TYR:HA   | 1:A:98:ILE:H     | 9                   | 0.41     | 0.16                | 0.45       |
| (1,407)  | 1:A:104:HIS:HA   | 1:A:105:GLU:H    | 9                   | 0.41     | 0.07                | 0.43       |
| (1,1274) | 1:B:104:HIS:HA   | 1:B:105:GLU:H    | 9                   | 0.41     | 0.07                | 0.43       |
| (1,218)  | 1:A:86:PRO:HB2   | 1:A:85:SER:HA    | 9                   | 0.38     | 0.07                | 0.4        |
| (1,218)  | 1:A:86:PRO:HB3   | 1:A:85:SER:HA    | 9                   | 0.38     | 0.07                | 0.4        |
| (1,1085) | 1:B:86:PRO:HB2   | 1:B:85:SER:HA    | 9                   | 0.38     | 0.07                | 0.4        |
| (1,1085) | 1:B:86:PRO:HB3   | 1:B:85:SER:HA    | 9                   | 0.38     | 0.07                | 0.4        |
| (1,231)  | 1:A:87:GLU:HB2   | 1:A:89:LEU:H     | 9                   | 0.38     | 0.11                | 0.42       |
| (1,231)  | 1:A:87:GLU:HB3   | 1:A:89:LEU:H     | 9                   | 0.38     | 0.11                | 0.42       |
| (1,489)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 9                   | 0.38     | 0.05                | 0.38       |
| (1,491)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 9                   | 0.38     | 0.05                | 0.38       |
| (1,239)  | 1:A:89:LEU:H     | 1:A:87:GLU:HA    | 9                   | 0.38     | 0.15                | 0.4        |
| (1,1098) | 1:B:87:GLU:HB2   | 1:B:89:LEU:H     | 9                   | 0.38     | 0.11                | 0.42       |
| (1,1098) | 1:B:87:GLU:HB3   | 1:B:89:LEU:H     | 9                   | 0.38     | 0.11                | 0.42       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1106) | 1:B:89:LEU:H     | 1:B:87:GLU:HA    | 9                   | 0.38     | 0.15                | 0.4        |
| (1,913)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HB2   | 9                   | 0.38     | 0.04                | 0.38       |
| (1,585)  | 1:A:121:LYS:HG2  | 1:A:121:LYS:HA   | 9                   | 0.38     | 0.04                | 0.39       |
| (1,585)  | 1:A:121:LYS:HG3  | 1:A:121:LYS:HA   | 9                   | 0.38     | 0.04                | 0.39       |
| (1,1452) | 1:B:121:LYS:HG2  | 1:B:121:LYS:HA   | 9                   | 0.38     | 0.04                | 0.39       |
| (1,1452) | 1:B:121:LYS:HG3  | 1:B:121:LYS:HA   | 9                   | 0.38     | 0.04                | 0.39       |
| (1,1356) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3  | 9                   | 0.38     | 0.05                | 0.38       |
| (1,1358) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3  | 9                   | 0.38     | 0.05                | 0.38       |
| (1,46)   | 1:A:75:PHE:HA    | 1:A:75:PHE:HB2   | 9                   | 0.38     | 0.05                | 0.38       |
| (1,1204) | 1:B:98:ILE:HD11  | 1:B:98:ILE:HB    | 9                   | 0.38     | 0.06                | 0.41       |
| (1,1204) | 1:B:98:ILE:HD12  | 1:B:98:ILE:HB    | 9                   | 0.38     | 0.06                | 0.41       |
| (1,1204) | 1:B:98:ILE:HD13  | 1:B:98:ILE:HB    | 9                   | 0.38     | 0.06                | 0.41       |
| (1,337)  | 1:A:98:ILE:HD11  | 1:A:98:ILE:HB    | 9                   | 0.36     | 0.06                | 0.32       |
| (1,337)  | 1:A:98:ILE:HD12  | 1:A:98:ILE:HB    | 9                   | 0.36     | 0.06                | 0.32       |
| (1,337)  | 1:A:98:ILE:HD13  | 1:A:98:ILE:HB    | 9                   | 0.36     | 0.06                | 0.32       |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB2  | 9                   | 0.36     | 0.1                 | 0.4        |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB3  | 9                   | 0.36     | 0.1                 | 0.4        |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB2  | 9                   | 0.36     | 0.09                | 0.4        |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB3  | 9                   | 0.36     | 0.09                | 0.4        |
| (1,578)  | 1:A:119:HIS:HA   | 1:A:119:HIS:H    | 9                   | 0.35     | 0.03                | 0.35       |
| (1,1445) | 1:B:119:HIS:HA   | 1:B:119:HIS:H    | 9                   | 0.35     | 0.03                | 0.35       |
| (1,804)  | 1:A:144:THR:HA   | 1:A:145:VAL:H    | 9                   | 0.35     | 0.02                | 0.36       |
| (1,1671) | 1:B:144:THR:HA   | 1:B:145:VAL:H    | 9                   | 0.35     | 0.02                | 0.36       |
| (1,647)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD11 | 9                   | 0.33     | 0.06                | 0.36       |
| (1,647)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD12 | 9                   | 0.33     | 0.06                | 0.36       |
| (1,647)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD13 | 9                   | 0.33     | 0.06                | 0.36       |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD11 | 9                   | 0.33     | 0.06                | 0.36       |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD12 | 9                   | 0.33     | 0.06                | 0.36       |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD13 | 9                   | 0.33     | 0.06                | 0.36       |
| (1,1586) | 1:B:133:ILE:HG21 | 1:B:133:ILE:HA   | 9                   | 0.32     | 0.04                | 0.33       |
| (1,1586) | 1:B:133:ILE:HG22 | 1:B:133:ILE:HA   | 9                   | 0.32     | 0.04                | 0.33       |
| (1,1586) | 1:B:133:ILE:HG23 | 1:B:133:ILE:HA   | 9                   | 0.32     | 0.04                | 0.33       |
| (1,719)  | 1:A:133:ILE:HG21 | 1:A:133:ILE:HA   | 9                   | 0.32     | 0.04                | 0.33       |
| (1,719)  | 1:A:133:ILE:HG22 | 1:A:133:ILE:HA   | 9                   | 0.32     | 0.04                | 0.33       |
| (1,719)  | 1:A:133:ILE:HG23 | 1:A:133:ILE:HA   | 9                   | 0.32     | 0.04                | 0.33       |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG11 | 9                   | 0.32     | 0.02                | 0.32       |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG12 | 9                   | 0.32     | 0.02                | 0.32       |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG13 | 9                   | 0.32     | 0.02                | 0.32       |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG21 | 9                   | 0.32     | 0.02                | 0.32       |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG22 | 9                   | 0.32     | 0.02                | 0.32       |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG23 | 9                   | 0.32     | 0.02                | 0.32       |
| (1,995)  | 1:B:78:ASN:HA    | 1:B:79:LEU:H     | 9                   | 0.32     | 0.05                | 0.34       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,128)  | 1:A:78:ASN:HA   | 1:A:79:LEU:H     | 9                   | 0.31     | 0.05                | 0.34       |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG11 | 9                   | 0.31     | 0.01                | 0.31       |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG12 | 9                   | 0.31     | 0.01                | 0.31       |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG13 | 9                   | 0.31     | 0.01                | 0.31       |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG21 | 9                   | 0.31     | 0.01                | 0.31       |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG22 | 9                   | 0.31     | 0.01                | 0.31       |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG23 | 9                   | 0.31     | 0.01                | 0.31       |
| (1,226)  | 1:A:87:GLU:HG2  | 1:A:88:GLU:H     | 9                   | 0.31     | 0.03                | 0.31       |
| (1,226)  | 1:A:87:GLU:HG3  | 1:A:88:GLU:H     | 9                   | 0.31     | 0.03                | 0.31       |
| (1,1093) | 1:B:87:GLU:HG2  | 1:B:88:GLU:H     | 9                   | 0.31     | 0.03                | 0.31       |
| (1,1093) | 1:B:87:GLU:HG3  | 1:B:88:GLU:H     | 9                   | 0.31     | 0.03                | 0.31       |
| (1,682)  | 1:A:129:ASP:H   | 1:A:128:VAL:HA   | 9                   | 0.3      | 0.03                | 0.31       |
| (1,1120) | 1:B:89:LEU:HA   | 1:B:90:LYS:H     | 9                   | 0.3      | 0.05                | 0.32       |
| (1,1549) | 1:B:129:ASP:H   | 1:B:128:VAL:HA   | 9                   | 0.3      | 0.03                | 0.31       |
| (1,253)  | 1:A:89:LEU:HA   | 1:A:90:LYS:H     | 9                   | 0.3      | 0.05                | 0.32       |
| (1,1517) | 1:B:125:PRO:HD3 | 1:B:124:ILE:HB   | 9                   | 0.28     | 0.05                | 0.3        |
| (1,650)  | 1:A:125:PRO:HD3 | 1:A:124:ILE:HB   | 9                   | 0.28     | 0.05                | 0.29       |
| (1,854)  | 1:A:148:PRO:HB2 | 1:A:149:ARG:H    | 9                   | 0.27     | 0.12                | 0.25       |
| (1,854)  | 1:A:148:PRO:HB3 | 1:A:149:ARG:H    | 9                   | 0.27     | 0.12                | 0.25       |
| (1,1721) | 1:B:148:PRO:HB2 | 1:B:149:ARG:H    | 9                   | 0.27     | 0.12                | 0.25       |
| (1,1721) | 1:B:148:PRO:HB3 | 1:B:149:ARG:H    | 9                   | 0.27     | 0.12                | 0.25       |
| (1,351)  | 1:A:99:GLU:HA   | 1:A:99:GLU:H     | 9                   | 0.27     | 0.05                | 0.27       |
| (1,1218) | 1:B:99:GLU:HA   | 1:B:99:GLU:H     | 9                   | 0.27     | 0.05                | 0.27       |
| (1,546)  | 1:A:117:GLU:HA  | 1:A:117:GLU:H    | 9                   | 0.26     | 0.03                | 0.26       |
| (1,1635) | 1:B:141:GLY:H   | 1:B:140:ASP:H    | 9                   | 0.26     | 0.06                | 0.23       |
| (1,1637) | 1:B:141:GLY:H   | 1:B:140:ASP:H    | 9                   | 0.26     | 0.06                | 0.23       |
| (1,1413) | 1:B:117:GLU:HA  | 1:B:117:GLU:H    | 9                   | 0.26     | 0.03                | 0.26       |
| (1,768)  | 1:A:141:GLY:H   | 1:A:140:ASP:H    | 9                   | 0.26     | 0.05                | 0.23       |
| (1,770)  | 1:A:141:GLY:H   | 1:A:140:ASP:H    | 9                   | 0.26     | 0.05                | 0.23       |
| (1,5)    | 1:A:67:GLU:H    | 1:A:67:GLU:HA    | 9                   | 0.26     | 0.06                | 0.28       |
| (1,872)  | 1:B:67:GLU:H    | 1:B:67:GLU:HA    | 9                   | 0.26     | 0.06                | 0.28       |
| (1,771)  | 1:A:141:GLY:HA2 | 1:A:141:GLY:H    | 9                   | 0.26     | 0.03                | 0.26       |
| (1,1638) | 1:B:141:GLY:HA2 | 1:B:141:GLY:H    | 9                   | 0.26     | 0.03                | 0.26       |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG11  | 9                   | 0.25     | 0.1                 | 0.2        |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG12  | 9                   | 0.25     | 0.1                 | 0.2        |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG13  | 9                   | 0.25     | 0.1                 | 0.2        |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG21  | 9                   | 0.25     | 0.1                 | 0.2        |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG22  | 9                   | 0.25     | 0.1                 | 0.2        |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG23  | 9                   | 0.25     | 0.1                 | 0.2        |
| (1,305)  | 1:A:95:GLY:HA2  | 1:A:96:ASP:H     | 9                   | 0.25     | 0.03                | 0.24       |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG11  | 9                   | 0.25     | 0.1                 | 0.19       |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG12  | 9                   | 0.25     | 0.1                 | 0.19       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG13 | 9                   | 0.25     | 0.1                 | 0.19       |
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG21 | 9                   | 0.25     | 0.1                 | 0.19       |
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG22 | 9                   | 0.25     | 0.1                 | 0.19       |
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG23 | 9                   | 0.25     | 0.1                 | 0.19       |
| (1,1172) | 1:B:95:GLY:HA2   | 1:B:96:ASP:H    | 9                   | 0.25     | 0.03                | 0.24       |
| (1,174)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB3  | 9                   | 0.24     | 0.04                | 0.24       |
| (1,175)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB3  | 9                   | 0.24     | 0.04                | 0.24       |
| (1,1041) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3  | 9                   | 0.24     | 0.04                | 0.24       |
| (1,1042) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3  | 9                   | 0.24     | 0.04                | 0.24       |
| (1,272)  | 1:A:92:LYS:H     | 1:A:91:VAL:HA   | 9                   | 0.23     | 0.02                | 0.23       |
| (1,1139) | 1:B:92:LYS:H     | 1:B:91:VAL:HA   | 9                   | 0.23     | 0.02                | 0.23       |
| (1,360)  | 1:A:100:VAL:HA   | 1:A:100:VAL:H   | 9                   | 0.22     | 0.04                | 0.23       |
| (1,1227) | 1:B:100:VAL:HA   | 1:B:100:VAL:H   | 9                   | 0.22     | 0.03                | 0.23       |
| (1,816)  | 1:A:145:VAL:HA   | 1:A:145:VAL:H   | 9                   | 0.2      | 0.01                | 0.2        |
| (1,822)  | 1:A:145:VAL:HA   | 1:A:146:ASP:H   | 9                   | 0.2      | 0.02                | 0.21       |
| (1,276)  | 1:A:92:LYS:H     | 1:A:92:LYS:HA   | 9                   | 0.2      | 0.02                | 0.2        |
| (1,1143) | 1:B:92:LYS:H     | 1:B:92:LYS:HA   | 9                   | 0.2      | 0.02                | 0.2        |
| (1,1689) | 1:B:145:VAL:HA   | 1:B:146:ASP:H   | 9                   | 0.2      | 0.02                | 0.21       |
| (1,1683) | 1:B:145:VAL:HA   | 1:B:145:VAL:H   | 9                   | 0.2      | 0.01                | 0.2        |
| (1,339)  | 1:A:98:ILE:HB    | 1:A:98:ILE:H    | 9                   | 0.19     | 0.04                | 0.19       |
| (1,1206) | 1:B:98:ILE:HB    | 1:B:98:ILE:H    | 9                   | 0.19     | 0.04                | 0.19       |
| (1,670)  | 1:A:127:ASP:HB3  | 1:A:127:ASP:H   | 9                   | 0.18     | 0.02                | 0.19       |
| (1,1537) | 1:B:127:ASP:HB3  | 1:B:127:ASP:H   | 9                   | 0.18     | 0.02                | 0.18       |
| (1,148)  | 1:A:80:ASP:H     | 1:A:80:ASP:HB3  | 9                   | 0.18     | 0.02                | 0.17       |
| (1,832)  | 1:A:146:ASP:HB2  | 1:A:146:ASP:HA  | 9                   | 0.18     | 0.02                | 0.18       |
| (1,835)  | 1:A:146:ASP:HB2  | 1:A:146:ASP:HA  | 9                   | 0.18     | 0.02                | 0.18       |
| (1,1015) | 1:B:80:ASP:H     | 1:B:80:ASP:HB3  | 9                   | 0.18     | 0.02                | 0.17       |
| (1,1699) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 9                   | 0.18     | 0.02                | 0.18       |
| (1,1702) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 9                   | 0.18     | 0.02                | 0.18       |
| (1,850)  | 1:A:147:GLY:HA2  | 1:A:149:ARG:H   | 8                   | 2.28     | 0.56                | 2.48       |
| (1,1717) | 1:B:147:GLY:HA2  | 1:B:149:ARG:H   | 8                   | 2.28     | 0.56                | 2.48       |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG2 | 8                   | 1.78     | 0.47                | 1.66       |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG3 | 8                   | 1.78     | 0.47                | 1.66       |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG2 | 8                   | 1.78     | 0.47                | 1.66       |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG3 | 8                   | 1.78     | 0.47                | 1.66       |
| (1,501)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HE1 | 8                   | 1.77     | 0.73                | 1.84       |
| (1,501)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HE1 | 8                   | 1.77     | 0.73                | 1.84       |
| (1,501)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HE1 | 8                   | 1.77     | 0.73                | 1.84       |
| (1,1368) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HE1 | 8                   | 1.77     | 0.73                | 1.84       |
| (1,1368) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HE1 | 8                   | 1.77     | 0.73                | 1.84       |
| (1,1368) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HE1 | 8                   | 1.77     | 0.73                | 1.84       |
| (1,22)   | 1:A:70:LEU:HB3   | 1:A:74:ARG:H    | 8                   | 1.74     | 0.85                | 1.86       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,889)  | 1:B:70:LEU:HB3   | 1:B:74:ARG:H     | 8                   | 1.73     | 0.85                | 1.85       |
| (1,385)  | 1:A:102:GLY:HA2  | 1:A:84:PHE:HZ    | 8                   | 1.65     | 0.74                | 1.79       |
| (1,1252) | 1:B:102:GLY:HA2  | 1:B:84:PHE:HZ    | 8                   | 1.65     | 0.74                | 1.8        |
| (1,1288) | 1:B:107:ARG:HD2  | 1:B:105:GLU:H    | 8                   | 1.54     | 0.6                 | 1.61       |
| (1,421)  | 1:A:107:ARG:HD2  | 1:A:105:GLU:H    | 8                   | 1.54     | 0.6                 | 1.6        |
| (1,502)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HB2  | 8                   | 1.34     | 0.78                | 1.42       |
| (1,502)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HB2  | 8                   | 1.34     | 0.78                | 1.42       |
| (1,502)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HB2  | 8                   | 1.34     | 0.78                | 1.42       |
| (1,1369) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HB2  | 8                   | 1.34     | 0.78                | 1.42       |
| (1,1369) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HB2  | 8                   | 1.34     | 0.78                | 1.42       |
| (1,1369) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HB2  | 8                   | 1.34     | 0.78                | 1.42       |
| (1,1767) | 1:A:122:TYR:HB2  | 1:B:112:GLY:HA3  | 8                   | 1.26     | 0.73                | 1.02       |
| (1,1767) | 1:A:122:TYR:HB3  | 1:B:112:GLY:HA3  | 8                   | 1.26     | 0.73                | 1.02       |
| (1,20)   | 1:A:70:LEU:HB3   | 1:A:71:GLU:H     | 8                   | 1.15     | 0.31                | 1.32       |
| (1,887)  | 1:B:70:LEU:HB3   | 1:B:71:GLU:H     | 8                   | 1.15     | 0.31                | 1.32       |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG21 | 8                   | 1.13     | 0.1                 | 1.09       |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG22 | 8                   | 1.13     | 0.1                 | 1.09       |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG23 | 8                   | 1.13     | 0.1                 | 1.09       |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG21 | 8                   | 1.13     | 0.1                 | 1.09       |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG22 | 8                   | 1.13     | 0.1                 | 1.09       |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG23 | 8                   | 1.13     | 0.1                 | 1.09       |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD11  | 8                   | 1.0      | 0.28                | 1.04       |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD12  | 8                   | 1.0      | 0.28                | 1.04       |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD13  | 8                   | 1.0      | 0.28                | 1.04       |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD11  | 8                   | 1.0      | 0.28                | 1.04       |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD12  | 8                   | 1.0      | 0.28                | 1.04       |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD13  | 8                   | 1.0      | 0.28                | 1.04       |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD11  | 8                   | 0.99     | 0.28                | 1.03       |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD12  | 8                   | 0.99     | 0.28                | 1.03       |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD13  | 8                   | 0.99     | 0.28                | 1.03       |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD11  | 8                   | 0.99     | 0.28                | 1.03       |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD12  | 8                   | 0.99     | 0.28                | 1.03       |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD13  | 8                   | 0.99     | 0.28                | 1.03       |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB2  | 8                   | 0.97     | 0.27                | 1.1        |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB3  | 8                   | 0.97     | 0.27                | 1.1        |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB2  | 8                   | 0.97     | 0.27                | 1.1        |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB3  | 8                   | 0.97     | 0.27                | 1.1        |
| (1,861)  | 1:A:150:LYS:HA   | 1:A:151:GLN:H    | 8                   | 0.9      | 0.08                | 0.9        |
| (1,1728) | 1:B:150:LYS:HA   | 1:B:151:GLN:H    | 8                   | 0.9      | 0.08                | 0.9        |
| (1,1770) | 1:A:123:ARG:HD2  | 1:B:113:PHE:H    | 8                   | 0.86     | 0.78                | 0.65       |
| (1,1770) | 1:A:123:ARG:HD3  | 1:B:113:PHE:H    | 8                   | 0.86     | 0.78                | 0.65       |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG2   | 8                   | 0.83     | 0.28                | 0.88       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG3  | 8                   | 0.83     | 0.28                | 0.88       |
| (1,564)  | 1:A:118:PHE:HD1  | 1:A:118:PHE:H   | 8                   | 0.83     | 0.43                | 0.81       |
| (1,564)  | 1:A:118:PHE:HD2  | 1:A:118:PHE:H   | 8                   | 0.83     | 0.43                | 0.81       |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG2  | 8                   | 0.83     | 0.28                | 0.88       |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG3  | 8                   | 0.83     | 0.28                | 0.88       |
| (1,1431) | 1:B:118:PHE:HD1  | 1:B:118:PHE:H   | 8                   | 0.82     | 0.43                | 0.81       |
| (1,1431) | 1:B:118:PHE:HD2  | 1:B:118:PHE:H   | 8                   | 0.82     | 0.43                | 0.81       |
| (1,167)  | 1:A:81:VAL:H     | 1:A:141:GLY:HA2 | 8                   | 0.81     | 0.62                | 0.52       |
| (1,1034) | 1:B:81:VAL:H     | 1:B:141:GLY:HA2 | 8                   | 0.81     | 0.62                | 0.52       |
| (1,480)  | 1:A:112:GLY:HA3  | 1:A:113:PHE:H   | 8                   | 0.8      | 0.07                | 0.82       |
| (1,1347) | 1:B:112:GLY:HA3  | 1:B:113:PHE:H   | 8                   | 0.8      | 0.07                | 0.82       |
| (1,115)  | 1:A:77:VAL:HG11  | 1:A:145:VAL:H   | 8                   | 0.79     | 0.79                | 0.39       |
| (1,115)  | 1:A:77:VAL:HG12  | 1:A:145:VAL:H   | 8                   | 0.79     | 0.79                | 0.39       |
| (1,115)  | 1:A:77:VAL:HG13  | 1:A:145:VAL:H   | 8                   | 0.79     | 0.79                | 0.39       |
| (1,982)  | 1:B:77:VAL:HG11  | 1:B:145:VAL:H   | 8                   | 0.79     | 0.79                | 0.39       |
| (1,982)  | 1:B:77:VAL:HG12  | 1:B:145:VAL:H   | 8                   | 0.79     | 0.79                | 0.39       |
| (1,982)  | 1:B:77:VAL:HG13  | 1:B:145:VAL:H   | 8                   | 0.79     | 0.79                | 0.39       |
| (1,710)  | 1:A:132:THR:HB   | 1:A:148:PRO:HD2 | 8                   | 0.76     | 0.11                | 0.8        |
| (1,710)  | 1:A:132:THR:HB   | 1:A:148:PRO:HD3 | 8                   | 0.76     | 0.11                | 0.8        |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD2 | 8                   | 0.76     | 0.11                | 0.8        |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD3 | 8                   | 0.76     | 0.11                | 0.8        |
| (1,855)  | 1:A:149:ARG:HB2  | 1:A:149:ARG:H   | 8                   | 0.63     | 0.07                | 0.65       |
| (1,855)  | 1:A:149:ARG:HB3  | 1:A:149:ARG:H   | 8                   | 0.63     | 0.07                | 0.65       |
| (1,1722) | 1:B:149:ARG:HB2  | 1:B:149:ARG:H   | 8                   | 0.63     | 0.07                | 0.65       |
| (1,1722) | 1:B:149:ARG:HB3  | 1:B:149:ARG:H   | 8                   | 0.63     | 0.07                | 0.65       |
| (1,524)  | 1:A:115:SER:HB2  | 1:A:106:GLU:H   | 8                   | 0.6      | 0.18                | 0.6        |
| (1,1391) | 1:B:115:SER:HB2  | 1:B:106:GLU:H   | 8                   | 0.6      | 0.18                | 0.6        |
| (1,1050) | 1:B:83:HIS:H     | 1:B:84:PHE:H    | 8                   | 0.59     | 0.28                | 0.48       |
| (1,1051) | 1:B:83:HIS:H     | 1:B:84:PHE:H    | 8                   | 0.59     | 0.28                | 0.48       |
| (1,183)  | 1:A:83:HIS:H     | 1:A:84:PHE:H    | 8                   | 0.59     | 0.28                | 0.48       |
| (1,184)  | 1:A:83:HIS:H     | 1:A:84:PHE:H    | 8                   | 0.59     | 0.28                | 0.48       |
| (1,426)  | 1:A:107:ARG:HD2  | 1:A:107:ARG:H   | 8                   | 0.58     | 0.39                | 0.5        |
| (1,1293) | 1:B:107:ARG:HD2  | 1:B:107:ARG:H   | 8                   | 0.58     | 0.39                | 0.5        |
| (1,1026) | 1:B:81:VAL:H     | 1:B:82:LYS:H    | 8                   | 0.57     | 0.24                | 0.62       |
| (1,159)  | 1:A:81:VAL:H     | 1:A:82:LYS:H    | 8                   | 0.56     | 0.24                | 0.61       |
| (1,819)  | 1:A:145:VAL:HG21 | 1:A:145:VAL:H   | 8                   | 0.56     | 0.14                | 0.55       |
| (1,819)  | 1:A:145:VAL:HG22 | 1:A:145:VAL:H   | 8                   | 0.56     | 0.14                | 0.55       |
| (1,819)  | 1:A:145:VAL:HG23 | 1:A:145:VAL:H   | 8                   | 0.56     | 0.14                | 0.55       |
| (1,1686) | 1:B:145:VAL:HG21 | 1:B:145:VAL:H   | 8                   | 0.56     | 0.14                | 0.55       |
| (1,1686) | 1:B:145:VAL:HG22 | 1:B:145:VAL:H   | 8                   | 0.56     | 0.14                | 0.55       |
| (1,1686) | 1:B:145:VAL:HG23 | 1:B:145:VAL:H   | 8                   | 0.56     | 0.14                | 0.55       |
| (1,1027) | 1:B:81:VAL:H     | 1:B:82:LYS:H    | 8                   | 0.52     | 0.28                | 0.62       |

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| Key      | Atom-1           | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|----------------|---------------------|----------|---------------------|------------|
| (1,160)  | 1:A:81:VAL:H     | 1:A:82:LYS:H   | 8                   | 0.52     | 0.28                | 0.61       |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG2 | 8                   | 0.5      | 0.02                | 0.5        |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG3 | 8                   | 0.5      | 0.02                | 0.5        |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG2 | 8                   | 0.5      | 0.02                | 0.5        |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG3 | 8                   | 0.5      | 0.02                | 0.5        |
| (1,387)  | 1:A:102:GLY:HA3  | 1:A:102:GLY:H  | 8                   | 0.48     | 0.14                | 0.55       |
| (1,1254) | 1:B:102:GLY:HA3  | 1:B:102:GLY:H  | 8                   | 0.48     | 0.14                | 0.56       |
| (1,445)  | 1:A:108:GLN:HA   | 1:A:113:PHE:H  | 8                   | 0.45     | 0.23                | 0.4        |
| (1,1312) | 1:B:108:GLN:HA   | 1:B:113:PHE:H  | 8                   | 0.45     | 0.23                | 0.4        |
| (1,287)  | 1:A:93:VAL:HA    | 1:A:98:ILE:HA  | 8                   | 0.43     | 0.09                | 0.43       |
| (1,1154) | 1:B:93:VAL:HA    | 1:B:98:ILE:HA  | 8                   | 0.43     | 0.09                | 0.43       |
| (1,621)  | 1:A:124:ILE:HD11 | 1:A:123:ARG:HA | 8                   | 0.41     | 0.09                | 0.38       |
| (1,621)  | 1:A:124:ILE:HD12 | 1:A:123:ARG:HA | 8                   | 0.41     | 0.09                | 0.38       |
| (1,621)  | 1:A:124:ILE:HD13 | 1:A:123:ARG:HA | 8                   | 0.41     | 0.09                | 0.38       |
| (1,1488) | 1:B:124:ILE:HD11 | 1:B:123:ARG:HA | 8                   | 0.41     | 0.09                | 0.38       |
| (1,1488) | 1:B:124:ILE:HD12 | 1:B:123:ARG:HA | 8                   | 0.41     | 0.09                | 0.38       |
| (1,1488) | 1:B:124:ILE:HD13 | 1:B:123:ARG:HA | 8                   | 0.41     | 0.09                | 0.38       |
| (1,291)  | 1:A:94:LEU:HD11  | 1:A:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,291)  | 1:A:94:LEU:HD12  | 1:A:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,291)  | 1:A:94:LEU:HD13  | 1:A:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,291)  | 1:A:94:LEU:HD21  | 1:A:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,291)  | 1:A:94:LEU:HD22  | 1:A:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,291)  | 1:A:94:LEU:HD23  | 1:A:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,1158) | 1:B:94:LEU:HD11  | 1:B:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,1158) | 1:B:94:LEU:HD12  | 1:B:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,1158) | 1:B:94:LEU:HD13  | 1:B:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,1158) | 1:B:94:LEU:HD21  | 1:B:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,1158) | 1:B:94:LEU:HD22  | 1:B:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,1158) | 1:B:94:LEU:HD23  | 1:B:94:LEU:H   | 8                   | 0.41     | 0.16                | 0.52       |
| (1,173)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HD2 | 8                   | 0.4      | 0.19                | 0.44       |
| (1,1040) | 1:B:83:HIS:HA    | 1:B:83:HIS:HD2 | 8                   | 0.4      | 0.2                 | 0.46       |
| (1,1332) | 1:B:111:HIS:HB2  | 1:B:111:HIS:H  | 8                   | 0.36     | 0.12                | 0.39       |
| (1,465)  | 1:A:111:HIS:HB2  | 1:A:111:HIS:H  | 8                   | 0.36     | 0.12                | 0.38       |
| (1,673)  | 1:A:127:ASP:HB3  | 1:A:128:VAL:H  | 8                   | 0.35     | 0.09                | 0.38       |
| (1,1540) | 1:B:127:ASP:HB3  | 1:B:128:VAL:H  | 8                   | 0.35     | 0.09                | 0.38       |
| (1,285)  | 1:A:93:VAL:HG11  | 1:A:93:VAL:H   | 8                   | 0.35     | 0.06                | 0.35       |
| (1,285)  | 1:A:93:VAL:HG12  | 1:A:93:VAL:H   | 8                   | 0.35     | 0.06                | 0.35       |
| (1,285)  | 1:A:93:VAL:HG13  | 1:A:93:VAL:H   | 8                   | 0.35     | 0.06                | 0.35       |
| (1,285)  | 1:A:93:VAL:HG21  | 1:A:93:VAL:H   | 8                   | 0.35     | 0.06                | 0.35       |
| (1,285)  | 1:A:93:VAL:HG22  | 1:A:93:VAL:H   | 8                   | 0.35     | 0.06                | 0.35       |
| (1,285)  | 1:A:93:VAL:HG23  | 1:A:93:VAL:H   | 8                   | 0.35     | 0.06                | 0.35       |
| (1,1152) | 1:B:93:VAL:HG11  | 1:B:93:VAL:H   | 8                   | 0.34     | 0.05                | 0.34       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1152) | 1:B:93:VAL:HG12 | 1:B:93:VAL:H    | 8                   | 0.34     | 0.05                | 0.34       |
| (1,1152) | 1:B:93:VAL:HG13 | 1:B:93:VAL:H    | 8                   | 0.34     | 0.05                | 0.34       |
| (1,1152) | 1:B:93:VAL:HG21 | 1:B:93:VAL:H    | 8                   | 0.34     | 0.05                | 0.34       |
| (1,1152) | 1:B:93:VAL:HG22 | 1:B:93:VAL:H    | 8                   | 0.34     | 0.05                | 0.34       |
| (1,1152) | 1:B:93:VAL:HG23 | 1:B:93:VAL:H    | 8                   | 0.34     | 0.05                | 0.34       |
| (1,306)  | 1:A:95:GLY:HA2  | 1:A:97:VAL:H    | 8                   | 0.33     | 0.04                | 0.32       |
| (1,1173) | 1:B:95:GLY:HA2  | 1:B:97:VAL:H    | 8                   | 0.33     | 0.04                | 0.32       |
| (1,378)  | 1:A:101:HIS:HB3 | 1:A:101:HIS:H   | 8                   | 0.3      | 0.07                | 0.3        |
| (1,1245) | 1:B:101:HIS:HB3 | 1:B:101:HIS:H   | 8                   | 0.3      | 0.06                | 0.3        |
| (1,252)  | 1:A:89:LEU:H    | 1:A:90:LYS:H    | 8                   | 0.3      | 0.11                | 0.26       |
| (1,1119) | 1:B:89:LEU:H    | 1:B:90:LYS:H    | 8                   | 0.3      | 0.11                | 0.26       |
| (1,1691) | 1:B:146:ASP:HB2 | 1:B:76:SER:HA   | 8                   | 0.26     | 0.07                | 0.29       |
| (1,1692) | 1:B:146:ASP:HB2 | 1:B:76:SER:HA   | 8                   | 0.26     | 0.07                | 0.29       |
| (1,824)  | 1:A:146:ASP:HB2 | 1:A:76:SER:HA   | 8                   | 0.26     | 0.07                | 0.29       |
| (1,825)  | 1:A:146:ASP:HB2 | 1:A:76:SER:HA   | 8                   | 0.26     | 0.07                | 0.29       |
| (1,278)  | 1:A:92:LYS:H    | 1:A:93:VAL:H    | 8                   | 0.26     | 0.03                | 0.26       |
| (1,1145) | 1:B:92:LYS:H    | 1:B:93:VAL:H    | 8                   | 0.26     | 0.03                | 0.26       |
| (1,51)   | 1:A:75:PHE:HA   | 1:A:76:SER:H    | 8                   | 0.24     | 0.07                | 0.29       |
| (1,918)  | 1:B:75:PHE:HA   | 1:B:76:SER:H    | 8                   | 0.24     | 0.07                | 0.29       |
| (1,591)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:HA  | 8                   | 0.22     | 0.07                | 0.21       |
| (1,591)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:HA  | 8                   | 0.22     | 0.07                | 0.21       |
| (1,593)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:HA  | 8                   | 0.22     | 0.07                | 0.21       |
| (1,593)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:HA  | 8                   | 0.22     | 0.07                | 0.21       |
| (1,1458) | 1:B:122:TYR:HB2 | 1:B:122:TYR:HA  | 8                   | 0.22     | 0.07                | 0.2        |
| (1,1458) | 1:B:122:TYR:HB3 | 1:B:122:TYR:HA  | 8                   | 0.22     | 0.07                | 0.2        |
| (1,1460) | 1:B:122:TYR:HB2 | 1:B:122:TYR:HA  | 8                   | 0.22     | 0.07                | 0.2        |
| (1,1460) | 1:B:122:TYR:HB3 | 1:B:122:TYR:HA  | 8                   | 0.22     | 0.07                | 0.2        |
| (1,680)  | 1:A:128:VAL:H   | 1:A:129:ASP:H   | 8                   | 0.21     | 0.09                | 0.18       |
| (1,1547) | 1:B:128:VAL:H   | 1:B:129:ASP:H   | 8                   | 0.21     | 0.09                | 0.18       |
| (1,454)  | 1:A:110:GLU:H   | 1:A:110:GLU:HA  | 8                   | 0.2      | 0.05                | 0.18       |
| (1,1321) | 1:B:110:GLU:H   | 1:B:110:GLU:HA  | 8                   | 0.2      | 0.05                | 0.18       |
| (1,1208) | 1:B:98:ILE:HB   | 1:B:99:GLU:H    | 8                   | 0.14     | 0.01                | 0.14       |
| (1,341)  | 1:A:98:ILE:HB   | 1:A:99:GLU:H    | 8                   | 0.14     | 0.01                | 0.14       |
| (1,1189) | 1:B:97:VAL:HB   | 1:B:94:LEU:HA   | 7                   | 2.69     | 0.07                | 2.69       |
| (1,322)  | 1:A:97:VAL:HB   | 1:A:94:LEU:HA   | 7                   | 2.69     | 0.07                | 2.69       |
| (1,1032) | 1:B:81:VAL:HG21 | 1:B:118:PHE:HD1 | 7                   | 2.31     | 0.73                | 2.42       |
| (1,1032) | 1:B:81:VAL:HG21 | 1:B:118:PHE:HD2 | 7                   | 2.31     | 0.73                | 2.42       |
| (1,1032) | 1:B:81:VAL:HG22 | 1:B:118:PHE:HD1 | 7                   | 2.31     | 0.73                | 2.42       |
| (1,1032) | 1:B:81:VAL:HG22 | 1:B:118:PHE:HD2 | 7                   | 2.31     | 0.73                | 2.42       |
| (1,1032) | 1:B:81:VAL:HG23 | 1:B:118:PHE:HD1 | 7                   | 2.31     | 0.73                | 2.42       |
| (1,1032) | 1:B:81:VAL:HG23 | 1:B:118:PHE:HD2 | 7                   | 2.31     | 0.73                | 2.42       |
| (1,165)  | 1:A:81:VAL:HG21 | 1:A:118:PHE:HD1 | 7                   | 2.31     | 0.73                | 2.41       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD2  | 7                   | 2.31     | 0.73                | 2.41       |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD1  | 7                   | 2.31     | 0.73                | 2.41       |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD2  | 7                   | 2.31     | 0.73                | 2.41       |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD1  | 7                   | 2.31     | 0.73                | 2.41       |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD2  | 7                   | 2.31     | 0.73                | 2.41       |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB2   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB3   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB2   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB3   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB2   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB3   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB2   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB3   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB2   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB3   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB2   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB3   | 7                   | 1.43     | 0.36                | 1.57       |
| (1,1762) | 1:A:122:TYR:HB2  | 1:B:111:HIS:H    | 7                   | 1.35     | 0.89                | 0.77       |
| (1,1762) | 1:A:122:TYR:HB3  | 1:B:111:HIS:H    | 7                   | 1.35     | 0.89                | 0.77       |
| (1,99)   | 1:A:77:VAL:HG21  | 1:A:78:ASN:HB2   | 7                   | 1.19     | 0.08                | 1.23       |
| (1,99)   | 1:A:77:VAL:HG22  | 1:A:78:ASN:HB2   | 7                   | 1.19     | 0.08                | 1.23       |
| (1,99)   | 1:A:77:VAL:HG23  | 1:A:78:ASN:HB2   | 7                   | 1.19     | 0.08                | 1.23       |
| (1,966)  | 1:B:77:VAL:HG21  | 1:B:78:ASN:HB2   | 7                   | 1.19     | 0.08                | 1.23       |
| (1,966)  | 1:B:77:VAL:HG22  | 1:B:78:ASN:HB2   | 7                   | 1.19     | 0.08                | 1.23       |
| (1,966)  | 1:B:77:VAL:HG23  | 1:B:78:ASN:HB2   | 7                   | 1.19     | 0.08                | 1.23       |
| (1,119)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB3  | 7                   | 1.19     | 0.98                | 0.56       |
| (1,986)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB3  | 7                   | 1.19     | 0.98                | 0.56       |
| (1,109)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:H     | 7                   | 1.15     | 0.36                | 1.16       |
| (1,109)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:H     | 7                   | 1.15     | 0.36                | 1.16       |
| (1,109)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:H     | 7                   | 1.15     | 0.36                | 1.16       |
| (1,976)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:H     | 7                   | 1.15     | 0.36                | 1.16       |
| (1,976)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:H     | 7                   | 1.15     | 0.36                | 1.16       |
| (1,976)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:H     | 7                   | 1.15     | 0.36                | 1.16       |
| (1,516)  | 1:A:114:ILE:H    | 1:A:114:ILE:HG12 | 7                   | 1.11     | 0.23                | 1.15       |
| (1,1383) | 1:B:114:ILE:H    | 1:B:114:ILE:HG12 | 7                   | 1.11     | 0.23                | 1.16       |
| (1,507)  | 1:A:114:ILE:HD11 | 1:A:107:ARG:HD3  | 7                   | 1.1      | 0.07                | 1.11       |
| (1,507)  | 1:A:114:ILE:HD12 | 1:A:107:ARG:HD3  | 7                   | 1.1      | 0.07                | 1.11       |
| (1,507)  | 1:A:114:ILE:HD13 | 1:A:107:ARG:HD3  | 7                   | 1.1      | 0.07                | 1.11       |
| (1,1374) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HD3  | 7                   | 1.1      | 0.08                | 1.11       |
| (1,1374) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HD3  | 7                   | 1.1      | 0.08                | 1.11       |
| (1,1374) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HD3  | 7                   | 1.1      | 0.08                | 1.11       |
| (1,170)  | 1:A:83:HIS:H     | 1:A:81:VAL:HB    | 7                   | 1.01     | 0.43                | 1.09       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE1  | 7                   | 1.01     | 0.48                | 0.99       |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE2  | 7                   | 1.01     | 0.48                | 0.99       |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE1  | 7                   | 1.01     | 0.48                | 0.99       |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE2  | 7                   | 1.01     | 0.48                | 0.99       |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE1  | 7                   | 1.01     | 0.48                | 0.99       |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE2  | 7                   | 1.01     | 0.48                | 0.99       |
| (1,1037) | 1:B:83:HIS:H     | 1:B:81:VAL:HB   | 7                   | 1.01     | 0.43                | 1.09       |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE1  | 7                   | 1.0      | 0.48                | 0.99       |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE2  | 7                   | 1.0      | 0.48                | 0.99       |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE1  | 7                   | 1.0      | 0.48                | 0.99       |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE2  | 7                   | 1.0      | 0.48                | 0.99       |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE1  | 7                   | 1.0      | 0.48                | 0.99       |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE2  | 7                   | 1.0      | 0.48                | 0.99       |
| (1,734)  | 1:A:135:SER:H    | 1:A:134:THR:HB  | 7                   | 0.95     | 0.15                | 0.88       |
| (1,1601) | 1:B:135:SER:H    | 1:B:134:THR:HB  | 7                   | 0.95     | 0.15                | 0.88       |
| (1,568)  | 1:A:119:HIS:HB3  | 1:A:101:HIS:HA  | 7                   | 0.9      | 0.24                | 0.95       |
| (1,1435) | 1:B:119:HIS:HB3  | 1:B:101:HIS:HA  | 7                   | 0.89     | 0.24                | 0.95       |
| (1,236)  | 1:A:89:LEU:HD21  | 1:A:85:SER:HB3  | 7                   | 0.88     | 0.33                | 0.97       |
| (1,236)  | 1:A:89:LEU:HD22  | 1:A:85:SER:HB3  | 7                   | 0.88     | 0.33                | 0.97       |
| (1,236)  | 1:A:89:LEU:HD23  | 1:A:85:SER:HB3  | 7                   | 0.88     | 0.33                | 0.97       |
| (1,1103) | 1:B:89:LEU:HD21  | 1:B:85:SER:HB3  | 7                   | 0.88     | 0.34                | 0.97       |
| (1,1103) | 1:B:89:LEU:HD22  | 1:B:85:SER:HB3  | 7                   | 0.88     | 0.34                | 0.97       |
| (1,1103) | 1:B:89:LEU:HD23  | 1:B:85:SER:HB3  | 7                   | 0.88     | 0.34                | 0.97       |
| (1,1750) | 1:A:115:SER:HB2  | 1:B:119:HIS:HE1 | 7                   | 0.81     | 0.3                 | 0.85       |
| (1,550)  | 1:A:118:PHE:HE1  | 1:A:102:GLY:H   | 7                   | 0.71     | 0.32                | 0.69       |
| (1,550)  | 1:A:118:PHE:HE2  | 1:A:102:GLY:H   | 7                   | 0.71     | 0.32                | 0.69       |
| (1,1417) | 1:B:118:PHE:HE1  | 1:B:102:GLY:H   | 7                   | 0.71     | 0.32                | 0.69       |
| (1,1417) | 1:B:118:PHE:HE2  | 1:B:102:GLY:H   | 7                   | 0.71     | 0.32                | 0.69       |
| (1,143)  | 1:A:79:LEU:HG    | 1:A:80:ASP:H    | 7                   | 0.7      | 0.05                | 0.7        |
| (1,1010) | 1:B:79:LEU:HG    | 1:B:80:ASP:H    | 7                   | 0.7      | 0.05                | 0.7        |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG21 | 7                   | 0.66     | 0.29                | 0.76       |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG22 | 7                   | 0.66     | 0.29                | 0.76       |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG23 | 7                   | 0.66     | 0.29                | 0.76       |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG21 | 7                   | 0.66     | 0.29                | 0.75       |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG22 | 7                   | 0.66     | 0.29                | 0.75       |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG23 | 7                   | 0.66     | 0.29                | 0.75       |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG11 | 7                   | 0.66     | 0.03                | 0.66       |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG12 | 7                   | 0.66     | 0.03                | 0.66       |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG13 | 7                   | 0.66     | 0.03                | 0.66       |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG11 | 7                   | 0.66     | 0.03                | 0.66       |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG12 | 7                   | 0.66     | 0.03                | 0.66       |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG13 | 7                   | 0.66     | 0.03                | 0.66       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG11  | 7                   | 0.66     | 0.02                | 0.66       |
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG12  | 7                   | 0.66     | 0.02                | 0.66       |
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG13  | 7                   | 0.66     | 0.02                | 0.66       |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG11  | 7                   | 0.66     | 0.02                | 0.66       |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG12  | 7                   | 0.66     | 0.02                | 0.66       |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG13  | 7                   | 0.66     | 0.02                | 0.66       |
| (1,981)  | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG11 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,981)  | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG12 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,981)  | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG13 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,981)  | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG11 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,981)  | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG12 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,981)  | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG13 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,981)  | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG11 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,981)  | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG12 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,981)  | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG13 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG11 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG12 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG13 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG11 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG12 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG13 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG11 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG12 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG13 | 7                   | 0.65     | 0.39                | 0.55       |
| (1,393)  | 1:A:103:LYS:H   | 1:A:88:GLU:HG2   | 7                   | 0.64     | 0.2                 | 0.57       |
| (1,393)  | 1:A:103:LYS:H   | 1:A:88:GLU:HG3   | 7                   | 0.64     | 0.2                 | 0.57       |
| (1,1260) | 1:B:103:LYS:H   | 1:B:88:GLU:HG2   | 7                   | 0.63     | 0.2                 | 0.57       |
| (1,1260) | 1:B:103:LYS:H   | 1:B:88:GLU:HG3   | 7                   | 0.63     | 0.2                 | 0.57       |
| (1,195)  | 1:A:84:PHE:HD1  | 1:A:84:PHE:H     | 7                   | 0.62     | 0.46                | 0.49       |
| (1,195)  | 1:A:84:PHE:HD2  | 1:A:84:PHE:H     | 7                   | 0.62     | 0.46                | 0.49       |
| (1,1062) | 1:B:84:PHE:HD1  | 1:B:84:PHE:H     | 7                   | 0.62     | 0.46                | 0.49       |
| (1,1062) | 1:B:84:PHE:HD2  | 1:B:84:PHE:H     | 7                   | 0.62     | 0.46                | 0.49       |
| (1,97)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:H     | 7                   | 0.56     | 0.28                | 0.53       |
| (1,97)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:H     | 7                   | 0.56     | 0.28                | 0.53       |
| (1,97)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:H     | 7                   | 0.56     | 0.28                | 0.53       |
| (1,964)  | 1:B:77:VAL:HG21 | 1:B:77:VAL:H     | 7                   | 0.56     | 0.28                | 0.53       |
| (1,964)  | 1:B:77:VAL:HG22 | 1:B:77:VAL:H     | 7                   | 0.56     | 0.28                | 0.53       |
| (1,964)  | 1:B:77:VAL:HG23 | 1:B:77:VAL:H     | 7                   | 0.56     | 0.28                | 0.53       |
| (1,1024) | 1:B:81:VAL:HG21 | 1:B:81:VAL:H     | 7                   | 0.55     | 0.18                | 0.57       |
| (1,1024) | 1:B:81:VAL:HG22 | 1:B:81:VAL:H     | 7                   | 0.55     | 0.18                | 0.57       |
| (1,1024) | 1:B:81:VAL:HG23 | 1:B:81:VAL:H     | 7                   | 0.55     | 0.18                | 0.57       |
| (1,157)  | 1:A:81:VAL:HG21 | 1:A:81:VAL:H     | 7                   | 0.55     | 0.18                | 0.57       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,157)  | 1:A:81:VAL:HG22  | 1:A:81:VAL:H     | 7                   | 0.55     | 0.18                | 0.57       |
| (1,157)  | 1:A:81:VAL:HG23  | 1:A:81:VAL:H     | 7                   | 0.55     | 0.18                | 0.57       |
| (1,1063) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H     | 7                   | 0.52     | 0.09                | 0.57       |
| (1,1063) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H     | 7                   | 0.52     | 0.09                | 0.57       |
| (1,1065) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H     | 7                   | 0.52     | 0.09                | 0.57       |
| (1,1065) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H     | 7                   | 0.52     | 0.09                | 0.57       |
| (1,196)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 7                   | 0.51     | 0.1                 | 0.57       |
| (1,196)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 7                   | 0.51     | 0.1                 | 0.57       |
| (1,198)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 7                   | 0.51     | 0.1                 | 0.57       |
| (1,198)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 7                   | 0.51     | 0.1                 | 0.57       |
| (1,432)  | 1:A:107:ARG:HG2  | 1:A:108:GLN:H    | 7                   | 0.51     | 0.11                | 0.53       |
| (1,432)  | 1:A:107:ARG:HG3  | 1:A:108:GLN:H    | 7                   | 0.51     | 0.11                | 0.53       |
| (1,1299) | 1:B:107:ARG:HG2  | 1:B:108:GLN:H    | 7                   | 0.51     | 0.11                | 0.53       |
| (1,1299) | 1:B:107:ARG:HG3  | 1:B:108:GLN:H    | 7                   | 0.51     | 0.11                | 0.53       |
| (1,260)  | 1:A:89:LEU:HD21  | 1:A:103:LYS:H    | 7                   | 0.49     | 0.4                 | 0.19       |
| (1,260)  | 1:A:89:LEU:HD22  | 1:A:103:LYS:H    | 7                   | 0.49     | 0.4                 | 0.19       |
| (1,260)  | 1:A:89:LEU:HD23  | 1:A:103:LYS:H    | 7                   | 0.49     | 0.4                 | 0.19       |
| (1,1127) | 1:B:89:LEU:HD21  | 1:B:103:LYS:H    | 7                   | 0.48     | 0.4                 | 0.19       |
| (1,1127) | 1:B:89:LEU:HD22  | 1:B:103:LYS:H    | 7                   | 0.48     | 0.4                 | 0.19       |
| (1,1127) | 1:B:89:LEU:HD23  | 1:B:103:LYS:H    | 7                   | 0.48     | 0.4                 | 0.19       |
| (1,300)  | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB2   | 7                   | 0.47     | 0.07                | 0.46       |
| (1,300)  | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB3   | 7                   | 0.47     | 0.07                | 0.46       |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB2   | 7                   | 0.47     | 0.07                | 0.46       |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB3   | 7                   | 0.47     | 0.07                | 0.46       |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB2   | 7                   | 0.46     | 0.35                | 0.34       |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB3   | 7                   | 0.46     | 0.35                | 0.34       |
| (1,367)  | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB2   | 7                   | 0.46     | 0.35                | 0.34       |
| (1,367)  | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB3   | 7                   | 0.46     | 0.35                | 0.34       |
| (1,345)  | 1:A:98:ILE:H     | 1:A:122:TYR:H    | 7                   | 0.45     | 0.24                | 0.46       |
| (1,346)  | 1:A:98:ILE:H     | 1:A:122:TYR:H    | 7                   | 0.45     | 0.24                | 0.46       |
| (1,1212) | 1:B:98:ILE:H     | 1:B:122:TYR:H    | 7                   | 0.45     | 0.24                | 0.46       |
| (1,1213) | 1:B:98:ILE:H     | 1:B:122:TYR:H    | 7                   | 0.45     | 0.24                | 0.46       |
| (1,1385) | 1:B:114:ILE:HG21 | 1:B:114:ILE:H    | 7                   | 0.44     | 0.2                 | 0.34       |
| (1,1385) | 1:B:114:ILE:HG22 | 1:B:114:ILE:H    | 7                   | 0.44     | 0.2                 | 0.34       |
| (1,1385) | 1:B:114:ILE:HG23 | 1:B:114:ILE:H    | 7                   | 0.44     | 0.2                 | 0.34       |
| (1,518)  | 1:A:114:ILE:HG21 | 1:A:114:ILE:H    | 7                   | 0.44     | 0.21                | 0.34       |
| (1,518)  | 1:A:114:ILE:HG22 | 1:A:114:ILE:H    | 7                   | 0.44     | 0.21                | 0.34       |
| (1,518)  | 1:A:114:ILE:HG23 | 1:A:114:ILE:H    | 7                   | 0.44     | 0.21                | 0.34       |
| (1,811)  | 1:A:145:VAL:HB   | 1:A:77:VAL:HB    | 7                   | 0.44     | 0.16                | 0.4        |
| (1,1678) | 1:B:145:VAL:HB   | 1:B:77:VAL:HB    | 7                   | 0.44     | 0.17                | 0.4        |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD11 | 7                   | 0.43     | 0.1                 | 0.44       |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD12 | 7                   | 0.43     | 0.1                 | 0.44       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD13 | 7                   | 0.43     | 0.1                 | 0.44       |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD21 | 7                   | 0.43     | 0.1                 | 0.44       |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD22 | 7                   | 0.43     | 0.1                 | 0.44       |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD23 | 7                   | 0.43     | 0.1                 | 0.44       |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD11 | 7                   | 0.43     | 0.1                 | 0.44       |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD12 | 7                   | 0.43     | 0.1                 | 0.44       |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD13 | 7                   | 0.43     | 0.1                 | 0.44       |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD21 | 7                   | 0.43     | 0.1                 | 0.44       |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD22 | 7                   | 0.43     | 0.1                 | 0.44       |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD23 | 7                   | 0.43     | 0.1                 | 0.44       |
| (1,955)  | 1:B:77:VAL:HG11  | 1:B:76:SER:HA    | 7                   | 0.41     | 0.03                | 0.41       |
| (1,955)  | 1:B:77:VAL:HG12  | 1:B:76:SER:HA    | 7                   | 0.41     | 0.03                | 0.41       |
| (1,955)  | 1:B:77:VAL:HG13  | 1:B:76:SER:HA    | 7                   | 0.41     | 0.03                | 0.41       |
| (1,88)   | 1:A:77:VAL:HG11  | 1:A:76:SER:HA    | 7                   | 0.4      | 0.03                | 0.41       |
| (1,88)   | 1:A:77:VAL:HG12  | 1:A:76:SER:HA    | 7                   | 0.4      | 0.03                | 0.41       |
| (1,88)   | 1:A:77:VAL:HG13  | 1:A:76:SER:HA    | 7                   | 0.4      | 0.03                | 0.41       |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG2   | 7                   | 0.39     | 0.15                | 0.37       |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG3   | 7                   | 0.39     | 0.15                | 0.37       |
| (1,892)  | 1:B:71:GLU:H     | 1:B:71:GLU:HG2   | 7                   | 0.39     | 0.16                | 0.36       |
| (1,892)  | 1:B:71:GLU:H     | 1:B:71:GLU:HG3   | 7                   | 0.39     | 0.16                | 0.36       |
| (1,267)  | 1:A:90:LYS:HB2   | 1:A:101:HIS:HB3  | 7                   | 0.39     | 0.33                | 0.27       |
| (1,267)  | 1:A:90:LYS:HB3   | 1:A:101:HIS:HB3  | 7                   | 0.39     | 0.33                | 0.27       |
| (1,1134) | 1:B:90:LYS:HB2   | 1:B:101:HIS:HB3  | 7                   | 0.39     | 0.33                | 0.27       |
| (1,1134) | 1:B:90:LYS:HB3   | 1:B:101:HIS:HB3  | 7                   | 0.39     | 0.33                | 0.27       |
| (1,700)  | 1:A:132:THR:HG21 | 1:A:132:THR:H    | 7                   | 0.36     | 0.2                 | 0.43       |
| (1,700)  | 1:A:132:THR:HG22 | 1:A:132:THR:H    | 7                   | 0.36     | 0.2                 | 0.43       |
| (1,700)  | 1:A:132:THR:HG23 | 1:A:132:THR:H    | 7                   | 0.36     | 0.2                 | 0.43       |
| (1,1436) | 1:B:119:HIS:HA   | 1:B:101:HIS:HA   | 7                   | 0.35     | 0.16                | 0.37       |
| (1,569)  | 1:A:119:HIS:HA   | 1:A:101:HIS:HA   | 7                   | 0.35     | 0.16                | 0.37       |
| (1,468)  | 1:A:111:HIS:H    | 1:A:112:GLY:H    | 7                   | 0.34     | 0.13                | 0.38       |
| (1,1335) | 1:B:111:HIS:H    | 1:B:112:GLY:H    | 7                   | 0.34     | 0.13                | 0.38       |
| (1,289)  | 1:A:94:LEU:H     | 1:A:93:VAL:HB    | 7                   | 0.28     | 0.06                | 0.26       |
| (1,1156) | 1:B:94:LEU:H     | 1:B:93:VAL:HB    | 7                   | 0.28     | 0.05                | 0.26       |
| (1,469)  | 1:A:111:HIS:HB2  | 1:A:112:GLY:H    | 7                   | 0.28     | 0.09                | 0.26       |
| (1,1336) | 1:B:111:HIS:HB2  | 1:B:112:GLY:H    | 7                   | 0.28     | 0.09                | 0.26       |
| (1,225)  | 1:A:87:GLU:H     | 1:A:88:GLU:H     | 7                   | 0.27     | 0.1                 | 0.22       |
| (1,228)  | 1:A:87:GLU:H     | 1:A:88:GLU:H     | 7                   | 0.27     | 0.1                 | 0.22       |
| (1,1092) | 1:B:87:GLU:H     | 1:B:88:GLU:H     | 7                   | 0.27     | 0.1                 | 0.22       |
| (1,1095) | 1:B:87:GLU:H     | 1:B:88:GLU:H     | 7                   | 0.27     | 0.1                 | 0.22       |
| (1,827)  | 1:A:146:ASP:HB3  | 1:A:76:SER:HA    | 7                   | 0.27     | 0.07                | 0.27       |
| (1,1694) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA    | 7                   | 0.27     | 0.07                | 0.27       |
| (1,898)  | 1:B:73:ASP:H     | 1:B:72:LYS:HB2   | 7                   | 0.26     | 0.08                | 0.24       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,898)  | 1:B:73:ASP:H    | 1:B:72:LYS:HB3  | 7                   | 0.26     | 0.08                | 0.24       |
| (1,31)   | 1:A:73:ASP:H    | 1:A:72:LYS:HB2  | 7                   | 0.26     | 0.07                | 0.24       |
| (1,31)   | 1:A:73:ASP:H    | 1:A:72:LYS:HB3  | 7                   | 0.26     | 0.07                | 0.24       |
| (1,138)  | 1:A:79:LEU:HD11 | 1:A:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,138)  | 1:A:79:LEU:HD12 | 1:A:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,138)  | 1:A:79:LEU:HD13 | 1:A:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,138)  | 1:A:79:LEU:HD21 | 1:A:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,138)  | 1:A:79:LEU:HD22 | 1:A:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,138)  | 1:A:79:LEU:HD23 | 1:A:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,1005) | 1:B:79:LEU:HD11 | 1:B:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,1005) | 1:B:79:LEU:HD12 | 1:B:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,1005) | 1:B:79:LEU:HD13 | 1:B:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,1005) | 1:B:79:LEU:HD21 | 1:B:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,1005) | 1:B:79:LEU:HD22 | 1:B:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,1005) | 1:B:79:LEU:HD23 | 1:B:79:LEU:HA   | 7                   | 0.26     | 0.04                | 0.26       |
| (1,817)  | 1:A:145:VAL:HB  | 1:A:145:VAL:H   | 7                   | 0.24     | 0.05                | 0.23       |
| (1,1684) | 1:B:145:VAL:HB  | 1:B:145:VAL:H   | 7                   | 0.24     | 0.06                | 0.23       |
| (1,369)  | 1:A:101:HIS:H   | 1:A:100:VAL:HA  | 7                   | 0.23     | 0.06                | 0.24       |
| (1,1236) | 1:B:101:HIS:H   | 1:B:100:VAL:HA  | 7                   | 0.23     | 0.06                | 0.24       |
| (1,67)   | 1:A:76:SER:HB2  | 1:A:146:ASP:HB2 | 7                   | 0.23     | 0.05                | 0.25       |
| (1,70)   | 1:A:76:SER:HB2  | 1:A:146:ASP:HB2 | 7                   | 0.23     | 0.05                | 0.25       |
| (1,73)   | 1:A:76:SER:HB2  | 1:A:146:ASP:HB2 | 7                   | 0.23     | 0.05                | 0.25       |
| (1,934)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2 | 7                   | 0.23     | 0.05                | 0.25       |
| (1,937)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2 | 7                   | 0.23     | 0.05                | 0.25       |
| (1,940)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2 | 7                   | 0.23     | 0.05                | 0.25       |
| (1,74)   | 1:A:76:SER:HA   | 1:A:146:ASP:HA  | 7                   | 0.23     | 0.07                | 0.21       |
| (1,78)   | 1:A:76:SER:HA   | 1:A:146:ASP:HA  | 7                   | 0.23     | 0.07                | 0.21       |
| (1,749)  | 1:A:136:SER:HA  | 1:A:137:LEU:H   | 7                   | 0.23     | 0.05                | 0.25       |
| (1,941)  | 1:B:76:SER:HA   | 1:B:146:ASP:HA  | 7                   | 0.23     | 0.07                | 0.21       |
| (1,945)  | 1:B:76:SER:HA   | 1:B:146:ASP:HA  | 7                   | 0.23     | 0.07                | 0.21       |
| (1,1616) | 1:B:136:SER:HA  | 1:B:137:LEU:H   | 7                   | 0.23     | 0.05                | 0.25       |
| (1,411)  | 1:A:105:GLU:HB2 | 1:A:105:GLU:H   | 7                   | 0.21     | 0.06                | 0.21       |
| (1,411)  | 1:A:105:GLU:HB3 | 1:A:105:GLU:H   | 7                   | 0.21     | 0.06                | 0.21       |
| (1,1278) | 1:B:105:GLU:HB2 | 1:B:105:GLU:H   | 7                   | 0.21     | 0.06                | 0.2        |
| (1,1278) | 1:B:105:GLU:HB3 | 1:B:105:GLU:H   | 7                   | 0.21     | 0.06                | 0.2        |
| (1,28)   | 1:A:72:LYS:H    | 1:A:72:LYS:HA   | 7                   | 0.2      | 0.05                | 0.18       |
| (1,895)  | 1:B:72:LYS:H    | 1:B:72:LYS:HA   | 7                   | 0.2      | 0.05                | 0.18       |
| (1,103)  | 1:A:77:VAL:H    | 1:A:78:ASN:H    | 7                   | 0.17     | 0.05                | 0.16       |
| (1,970)  | 1:B:77:VAL:H    | 1:B:78:ASN:H    | 7                   | 0.17     | 0.05                | 0.16       |
| (1,606)  | 1:A:123:ARG:HB2 | 1:A:123:ARG:HD2 | 7                   | 0.16     | 0.02                | 0.17       |
| (1,606)  | 1:A:123:ARG:HB2 | 1:A:123:ARG:HD3 | 7                   | 0.16     | 0.02                | 0.17       |
| (1,1473) | 1:B:123:ARG:HB2 | 1:B:123:ARG:HD2 | 7                   | 0.16     | 0.02                | 0.17       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1473) | 1:B:123:ARG:HB2 | 1:B:123:ARG:HD3 | 7                   | 0.16     | 0.02                | 0.17       |
| (1,847)  | 1:A:147:GLY:HA2 | 1:A:147:GLY:H   | 7                   | 0.16     | 0.05                | 0.13       |
| (1,1714) | 1:B:147:GLY:HA2 | 1:B:147:GLY:H   | 7                   | 0.16     | 0.05                | 0.13       |
| (1,896)  | 1:B:72:LYS:HB2  | 1:B:72:LYS:H    | 7                   | 0.16     | 0.02                | 0.16       |
| (1,896)  | 1:B:72:LYS:HB3  | 1:B:72:LYS:H    | 7                   | 0.16     | 0.02                | 0.16       |
| (1,29)   | 1:A:72:LYS:HB2  | 1:A:72:LYS:H    | 7                   | 0.16     | 0.02                | 0.15       |
| (1,29)   | 1:A:72:LYS:HB3  | 1:A:72:LYS:H    | 7                   | 0.16     | 0.02                | 0.15       |
| (1,335)  | 1:A:98:ILE:H    | 1:A:97:VAL:H    | 7                   | 0.16     | 0.06                | 0.14       |
| (1,1202) | 1:B:98:ILE:H    | 1:B:97:VAL:H    | 7                   | 0.16     | 0.06                | 0.14       |
| (1,442)  | 1:A:108:GLN:HA  | 1:A:108:GLN:HB2 | 7                   | 0.13     | 0.01                | 0.14       |
| (1,442)  | 1:A:108:GLN:HA  | 1:A:108:GLN:HB3 | 7                   | 0.13     | 0.01                | 0.14       |
| (1,1309) | 1:B:108:GLN:HA  | 1:B:108:GLN:HB2 | 7                   | 0.13     | 0.01                | 0.14       |
| (1,1309) | 1:B:108:GLN:HA  | 1:B:108:GLN:HB3 | 7                   | 0.13     | 0.01                | 0.14       |
| (1,325)  | 1:A:97:VAL:HB   | 1:A:97:VAL:HA   | 7                   | 0.13     | 0.02                | 0.13       |
| (1,326)  | 1:A:97:VAL:HB   | 1:A:97:VAL:HA   | 7                   | 0.13     | 0.02                | 0.13       |
| (1,1192) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA   | 7                   | 0.13     | 0.01                | 0.13       |
| (1,1193) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA   | 7                   | 0.13     | 0.01                | 0.13       |
| (1,1018) | 1:B:81:VAL:HG11 | 1:B:79:LEU:HG   | 6                   | 2.03     | 1.32                | 2.06       |
| (1,1018) | 1:B:81:VAL:HG12 | 1:B:79:LEU:HG   | 6                   | 2.03     | 1.32                | 2.06       |
| (1,1018) | 1:B:81:VAL:HG13 | 1:B:79:LEU:HG   | 6                   | 2.03     | 1.32                | 2.06       |
| (1,151)  | 1:A:81:VAL:HG11 | 1:A:79:LEU:HG   | 6                   | 2.03     | 1.32                | 2.06       |
| (1,151)  | 1:A:81:VAL:HG12 | 1:A:79:LEU:HG   | 6                   | 2.03     | 1.32                | 2.06       |
| (1,151)  | 1:A:81:VAL:HG13 | 1:A:79:LEU:HG   | 6                   | 2.03     | 1.32                | 2.06       |
| (1,257)  | 1:A:89:LEU:HD11 | 1:A:102:GLY:HA2 | 6                   | 1.12     | 0.47                | 1.28       |
| (1,257)  | 1:A:89:LEU:HD12 | 1:A:102:GLY:HA2 | 6                   | 1.12     | 0.47                | 1.28       |
| (1,257)  | 1:A:89:LEU:HD13 | 1:A:102:GLY:HA2 | 6                   | 1.12     | 0.47                | 1.28       |
| (1,1124) | 1:B:89:LEU:HD11 | 1:B:102:GLY:HA2 | 6                   | 1.12     | 0.47                | 1.28       |
| (1,1124) | 1:B:89:LEU:HD12 | 1:B:102:GLY:HA2 | 6                   | 1.12     | 0.47                | 1.28       |
| (1,1124) | 1:B:89:LEU:HD13 | 1:B:102:GLY:HA2 | 6                   | 1.12     | 0.47                | 1.28       |
| (1,1264) | 1:B:103:LYS:HG2 | 1:B:116:ARG:H   | 6                   | 1.1      | 0.32                | 1.06       |
| (1,1264) | 1:B:103:LYS:HG3 | 1:B:116:ARG:H   | 6                   | 1.1      | 0.32                | 1.06       |
| (1,397)  | 1:A:103:LYS:HG2 | 1:A:116:ARG:H   | 6                   | 1.1      | 0.32                | 1.06       |
| (1,397)  | 1:A:103:LYS:HG3 | 1:A:116:ARG:H   | 6                   | 1.1      | 0.32                | 1.06       |
| (1,82)   | 1:A:77:VAL:HG21 | 1:A:68:MET:HA   | 6                   | 1.09     | 0.15                | 1.15       |
| (1,82)   | 1:A:77:VAL:HG22 | 1:A:68:MET:HA   | 6                   | 1.09     | 0.15                | 1.15       |
| (1,82)   | 1:A:77:VAL:HG23 | 1:A:68:MET:HA   | 6                   | 1.09     | 0.15                | 1.15       |
| (1,949)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HA   | 6                   | 1.09     | 0.15                | 1.14       |
| (1,949)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HA   | 6                   | 1.09     | 0.15                | 1.14       |
| (1,949)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HA   | 6                   | 1.09     | 0.15                | 1.14       |
| (1,880)  | 1:B:68:MET:HE1  | 1:B:122:TYR:HE1 | 6                   | 0.95     | 0.49                | 0.92       |
| (1,880)  | 1:B:68:MET:HE1  | 1:B:122:TYR:HE2 | 6                   | 0.95     | 0.49                | 0.92       |
| (1,880)  | 1:B:68:MET:HE2  | 1:B:122:TYR:HE1 | 6                   | 0.95     | 0.49                | 0.92       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,880)  | 1:B:68:MET:HE2   | 1:B:122:TYR:HE2 | 6                   | 0.95     | 0.49                | 0.92       |
| (1,880)  | 1:B:68:MET:HE3   | 1:B:122:TYR:HE1 | 6                   | 0.95     | 0.49                | 0.92       |
| (1,880)  | 1:B:68:MET:HE3   | 1:B:122:TYR:HE2 | 6                   | 0.95     | 0.49                | 0.92       |
| (1,365)  | 1:A:100:VAL:HG11 | 1:A:102:GLY:H   | 6                   | 0.95     | 0.25                | 1.04       |
| (1,365)  | 1:A:100:VAL:HG12 | 1:A:102:GLY:H   | 6                   | 0.95     | 0.25                | 1.04       |
| (1,365)  | 1:A:100:VAL:HG13 | 1:A:102:GLY:H   | 6                   | 0.95     | 0.25                | 1.04       |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE1 | 6                   | 0.95     | 0.49                | 0.92       |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE2 | 6                   | 0.95     | 0.49                | 0.92       |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE1 | 6                   | 0.95     | 0.49                | 0.92       |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE2 | 6                   | 0.95     | 0.49                | 0.92       |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE1 | 6                   | 0.95     | 0.49                | 0.92       |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE2 | 6                   | 0.95     | 0.49                | 0.92       |
| (1,1232) | 1:B:100:VAL:HG11 | 1:B:102:GLY:H   | 6                   | 0.95     | 0.25                | 1.04       |
| (1,1232) | 1:B:100:VAL:HG12 | 1:B:102:GLY:H   | 6                   | 0.95     | 0.25                | 1.04       |
| (1,1232) | 1:B:100:VAL:HG13 | 1:B:102:GLY:H   | 6                   | 0.95     | 0.25                | 1.04       |
| (1,563)  | 1:A:118:PHE:HB2  | 1:A:118:PHE:H   | 6                   | 0.93     | 0.27                | 1.04       |
| (1,1430) | 1:B:118:PHE:HB2  | 1:B:118:PHE:H   | 6                   | 0.93     | 0.27                | 1.04       |
| (1,953)  | 1:B:77:VAL:HG21  | 1:B:75:PHE:HZ   | 6                   | 0.92     | 0.2                 | 0.93       |
| (1,953)  | 1:B:77:VAL:HG22  | 1:B:75:PHE:HZ   | 6                   | 0.92     | 0.2                 | 0.93       |
| (1,953)  | 1:B:77:VAL:HG23  | 1:B:75:PHE:HZ   | 6                   | 0.92     | 0.2                 | 0.93       |
| (1,1472) | 1:B:123:ARG:HD2  | 1:B:98:ILE:H    | 6                   | 0.9      | 0.34                | 0.88       |
| (1,1472) | 1:B:123:ARG:HD3  | 1:B:98:ILE:H    | 6                   | 0.9      | 0.34                | 0.88       |
| (1,605)  | 1:A:123:ARG:HD2  | 1:A:98:ILE:H    | 6                   | 0.9      | 0.34                | 0.88       |
| (1,605)  | 1:A:123:ARG:HD3  | 1:A:98:ILE:H    | 6                   | 0.9      | 0.34                | 0.88       |
| (1,511)  | 1:A:114:ILE:HG21 | 1:A:112:GLY:H   | 6                   | 0.88     | 0.6                 | 0.68       |
| (1,511)  | 1:A:114:ILE:HG22 | 1:A:112:GLY:H   | 6                   | 0.88     | 0.6                 | 0.68       |
| (1,511)  | 1:A:114:ILE:HG23 | 1:A:112:GLY:H   | 6                   | 0.88     | 0.6                 | 0.68       |
| (1,1378) | 1:B:114:ILE:HG21 | 1:B:112:GLY:H   | 6                   | 0.88     | 0.6                 | 0.68       |
| (1,1378) | 1:B:114:ILE:HG22 | 1:B:112:GLY:H   | 6                   | 0.88     | 0.6                 | 0.68       |
| (1,1378) | 1:B:114:ILE:HG23 | 1:B:112:GLY:H   | 6                   | 0.88     | 0.6                 | 0.68       |
| (1,86)   | 1:A:77:VAL:HG21  | 1:A:75:PHE:HZ   | 6                   | 0.83     | 0.12                | 0.9        |
| (1,86)   | 1:A:77:VAL:HG22  | 1:A:75:PHE:HZ   | 6                   | 0.83     | 0.12                | 0.9        |
| (1,86)   | 1:A:77:VAL:HG23  | 1:A:75:PHE:HZ   | 6                   | 0.83     | 0.12                | 0.9        |
| (1,246)  | 1:A:89:LEU:H     | 1:A:89:LEU:HG   | 6                   | 0.82     | 0.16                | 0.86       |
| (1,1113) | 1:B:89:LEU:H     | 1:B:89:LEU:HG   | 6                   | 0.82     | 0.16                | 0.86       |
| (1,166)  | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD1 | 6                   | 0.78     | 0.33                | 0.74       |
| (1,166)  | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD2 | 6                   | 0.78     | 0.33                | 0.74       |
| (1,166)  | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD1 | 6                   | 0.78     | 0.33                | 0.74       |
| (1,166)  | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD2 | 6                   | 0.78     | 0.33                | 0.74       |
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD1 | 6                   | 0.78     | 0.33                | 0.74       |
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD2 | 6                   | 0.78     | 0.33                | 0.74       |
| (1,1033) | 1:B:81:VAL:HG11  | 1:B:118:PHE:HD1 | 6                   | 0.78     | 0.33                | 0.74       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1033) | 1:B:81:VAL:HG11  | 1:B:118:PHE:HD2 | 6                   | 0.78     | 0.33                | 0.74       |
| (1,1033) | 1:B:81:VAL:HG12  | 1:B:118:PHE:HD1 | 6                   | 0.78     | 0.33                | 0.74       |
| (1,1033) | 1:B:81:VAL:HG12  | 1:B:118:PHE:HD2 | 6                   | 0.78     | 0.33                | 0.74       |
| (1,1033) | 1:B:81:VAL:HG13  | 1:B:118:PHE:HD1 | 6                   | 0.78     | 0.33                | 0.74       |
| (1,1033) | 1:B:81:VAL:HG13  | 1:B:118:PHE:HD2 | 6                   | 0.78     | 0.33                | 0.74       |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD21 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD22 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD23 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD21 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD22 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD23 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD21 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD22 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD23 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD21 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD22 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD23 | 6                   | 0.74     | 0.37                | 0.56       |
| (1,203)  | 1:A:84:PHE:HE1   | 1:A:116:ARG:H   | 6                   | 0.69     | 0.61                | 0.36       |
| (1,203)  | 1:A:84:PHE:HE2   | 1:A:116:ARG:H   | 6                   | 0.69     | 0.61                | 0.36       |
| (1,1070) | 1:B:84:PHE:HE1   | 1:B:116:ARG:H   | 6                   | 0.69     | 0.6                 | 0.36       |
| (1,1070) | 1:B:84:PHE:HE2   | 1:B:116:ARG:H   | 6                   | 0.69     | 0.6                 | 0.36       |
| (1,111)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HE1 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,111)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HE2 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,111)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HE1 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,111)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HE2 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,111)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HE1 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,111)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HE2 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,978)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HE1 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,978)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HE2 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,978)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HE1 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,978)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HE2 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,978)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HE1 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,978)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HE2 | 6                   | 0.68     | 0.32                | 0.62       |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE1 | 6                   | 0.67     | 0.25                | 0.66       |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE2 | 6                   | 0.67     | 0.25                | 0.66       |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE1 | 6                   | 0.67     | 0.25                | 0.66       |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE2 | 6                   | 0.67     | 0.25                | 0.66       |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE1 | 6                   | 0.67     | 0.25                | 0.66       |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE2 | 6                   | 0.67     | 0.25                | 0.66       |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD11 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD12 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD13 | 6                   | 0.66     | 0.49                | 0.44       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD21 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD22 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD23 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD11 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD12 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD13 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD21 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD22 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD23 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD11 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD12 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD13 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD21 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD22 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD23 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE1  | 1:B:70:LEU:HD11 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE1  | 1:B:70:LEU:HD12 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE1  | 1:B:70:LEU:HD13 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE1  | 1:B:70:LEU:HD21 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE1  | 1:B:70:LEU:HD22 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE1  | 1:B:70:LEU:HD23 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD11 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD12 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD13 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD21 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD22 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD23 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD11 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD12 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD13 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD21 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD22 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD23 | 6                   | 0.66     | 0.49                | 0.44       |
| (1,831)  | 1:A:146:ASP:HB2 | 1:A:145:VAL:HA  | 6                   | 0.63     | 0.07                | 0.64       |
| (1,1698) | 1:B:146:ASP:HB2 | 1:B:145:VAL:HA  | 6                   | 0.63     | 0.07                | 0.64       |
| (1,355)  | 1:A:99:GLU:HB2  | 1:A:121:LYS:HG2 | 6                   | 0.61     | 0.18                | 0.68       |
| (1,355)  | 1:A:99:GLU:HB2  | 1:A:121:LYS:HG3 | 6                   | 0.61     | 0.18                | 0.68       |
| (1,355)  | 1:A:99:GLU:HB3  | 1:A:121:LYS:HG2 | 6                   | 0.61     | 0.18                | 0.68       |
| (1,355)  | 1:A:99:GLU:HB3  | 1:A:121:LYS:HG3 | 6                   | 0.61     | 0.18                | 0.68       |
| (1,1222) | 1:B:99:GLU:HB2  | 1:B:121:LYS:HG2 | 6                   | 0.61     | 0.18                | 0.68       |
| (1,1222) | 1:B:99:GLU:HB2  | 1:B:121:LYS:HG3 | 6                   | 0.61     | 0.18                | 0.68       |
| (1,1222) | 1:B:99:GLU:HB3  | 1:B:121:LYS:HG2 | 6                   | 0.61     | 0.18                | 0.68       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1222) | 1:B:99:GLU:HB3   | 1:B:121:LYS:HG3 | 6                   | 0.61     | 0.18                | 0.68       |
| (1,539)  | 1:A:116:ARG:H    | 1:A:116:ARG:HG2 | 6                   | 0.6      | 0.31                | 0.43       |
| (1,539)  | 1:A:116:ARG:H    | 1:A:116:ARG:HG3 | 6                   | 0.6      | 0.31                | 0.43       |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG2 | 6                   | 0.6      | 0.31                | 0.43       |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG3 | 6                   | 0.6      | 0.31                | 0.43       |
| (1,1482) | 1:B:124:ILE:HB   | 1:B:97:VAL:HA   | 6                   | 0.57     | 0.41                | 0.47       |
| (1,615)  | 1:A:124:ILE:HB   | 1:A:97:VAL:HA   | 6                   | 0.57     | 0.4                 | 0.47       |
| (1,543)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HA  | 6                   | 0.56     | 0.17                | 0.5        |
| (1,544)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HA  | 6                   | 0.56     | 0.17                | 0.5        |
| (1,1410) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA  | 6                   | 0.56     | 0.17                | 0.5        |
| (1,1411) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA  | 6                   | 0.56     | 0.17                | 0.5        |
| (1,579)  | 1:A:119:HIS:H    | 1:A:120:ARG:H   | 6                   | 0.54     | 0.17                | 0.52       |
| (1,1446) | 1:B:119:HIS:H    | 1:B:120:ARG:H   | 6                   | 0.54     | 0.17                | 0.52       |
| (1,158)  | 1:A:81:VAL:H     | 1:A:81:VAL:HB   | 6                   | 0.48     | 0.05                | 0.46       |
| (1,1025) | 1:B:81:VAL:H     | 1:B:81:VAL:HB   | 6                   | 0.48     | 0.05                | 0.46       |
| (1,212)  | 1:A:85:SER:HB2   | 1:A:88:GLU:H    | 6                   | 0.47     | 0.13                | 0.4        |
| (1,1079) | 1:B:85:SER:HB2   | 1:B:88:GLU:H    | 6                   | 0.47     | 0.13                | 0.4        |
| (1,108)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:H    | 6                   | 0.43     | 0.23                | 0.32       |
| (1,108)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:H    | 6                   | 0.43     | 0.23                | 0.32       |
| (1,108)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:H    | 6                   | 0.43     | 0.23                | 0.32       |
| (1,975)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:H    | 6                   | 0.43     | 0.23                | 0.32       |
| (1,975)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:H    | 6                   | 0.43     | 0.23                | 0.32       |
| (1,975)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:H    | 6                   | 0.43     | 0.23                | 0.32       |
| (1,1567) | 1:B:132:THR:HG21 | 1:B:132:THR:H   | 6                   | 0.4      | 0.18                | 0.45       |
| (1,1567) | 1:B:132:THR:HG22 | 1:B:132:THR:H   | 6                   | 0.4      | 0.18                | 0.45       |
| (1,1567) | 1:B:132:THR:HG23 | 1:B:132:THR:H   | 6                   | 0.4      | 0.18                | 0.45       |
| (1,574)  | 1:A:119:HIS:HB3  | 1:A:119:HIS:HD2 | 6                   | 0.39     | 0.04                | 0.39       |
| (1,1441) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HD2 | 6                   | 0.38     | 0.05                | 0.4        |
| (1,470)  | 1:A:111:HIS:HA   | 1:A:112:GLY:H   | 6                   | 0.36     | 0.1                 | 0.36       |
| (1,1337) | 1:B:111:HIS:HA   | 1:B:112:GLY:H   | 6                   | 0.36     | 0.1                 | 0.36       |
| (1,281)  | 1:A:92:LYS:H     | 1:A:101:HIS:H   | 6                   | 0.35     | 0.11                | 0.3        |
| (1,1148) | 1:B:92:LYS:H     | 1:B:101:HIS:H   | 6                   | 0.35     | 0.11                | 0.3        |
| (1,56)   | 1:A:75:PHE:HD1   | 1:A:148:PRO:HA  | 6                   | 0.35     | 0.22                | 0.3        |
| (1,56)   | 1:A:75:PHE:HD2   | 1:A:148:PRO:HA  | 6                   | 0.35     | 0.22                | 0.3        |
| (1,923)  | 1:B:75:PHE:HD1   | 1:B:148:PRO:HA  | 6                   | 0.35     | 0.22                | 0.3        |
| (1,923)  | 1:B:75:PHE:HD2   | 1:B:148:PRO:HA  | 6                   | 0.35     | 0.22                | 0.3        |
| (1,1649) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |
| (1,1649) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |
| (1,1649) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |
| (1,1649) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |
| (1,1649) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |
| (1,1649) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1650) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |
| (1,1650) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |
| (1,1650) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |
| (1,1650) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |
| (1,1650) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |
| (1,1650) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H   | 6                   | 0.34     | 0.14                | 0.37       |
| (1,809)  | 1:A:144:THR:HG21 | 1:A:146:ASP:HB3 | 6                   | 0.31     | 0.19                | 0.24       |
| (1,809)  | 1:A:144:THR:HG22 | 1:A:146:ASP:HB3 | 6                   | 0.31     | 0.19                | 0.24       |
| (1,809)  | 1:A:144:THR:HG23 | 1:A:146:ASP:HB3 | 6                   | 0.31     | 0.19                | 0.24       |
| (1,1676) | 1:B:144:THR:HG21 | 1:B:146:ASP:HB3 | 6                   | 0.3      | 0.19                | 0.24       |
| (1,1676) | 1:B:144:THR:HG22 | 1:B:146:ASP:HB3 | 6                   | 0.3      | 0.19                | 0.24       |
| (1,1676) | 1:B:144:THR:HG23 | 1:B:146:ASP:HB3 | 6                   | 0.3      | 0.19                | 0.24       |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD21 | 6                   | 0.28     | 0.1                 | 0.31       |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD22 | 6                   | 0.28     | 0.1                 | 0.31       |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD23 | 6                   | 0.28     | 0.1                 | 0.31       |
| (1,1112) | 1:B:89:LEU:HA    | 1:B:89:LEU:HD21 | 6                   | 0.28     | 0.1                 | 0.31       |
| (1,1112) | 1:B:89:LEU:HA    | 1:B:89:LEU:HD22 | 6                   | 0.28     | 0.1                 | 0.31       |
| (1,1112) | 1:B:89:LEU:HA    | 1:B:89:LEU:HD23 | 6                   | 0.28     | 0.1                 | 0.31       |
| (1,826)  | 1:A:146:ASP:HB3  | 1:A:76:SER:HA   | 6                   | 0.28     | 0.06                | 0.28       |
| (1,1693) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA   | 6                   | 0.28     | 0.06                | 0.28       |
| (1,745)  | 1:A:136:SER:H    | 1:A:135:SER:H   | 6                   | 0.27     | 0.03                | 0.27       |
| (1,1612) | 1:B:136:SER:H    | 1:B:135:SER:H   | 6                   | 0.27     | 0.03                | 0.27       |
| (1,430)  | 1:A:107:ARG:H    | 1:A:108:GLN:H   | 6                   | 0.26     | 0.11                | 0.22       |
| (1,1297) | 1:B:107:ARG:H    | 1:B:108:GLN:H   | 6                   | 0.26     | 0.11                | 0.22       |
| (1,1147) | 1:B:92:LYS:H     | 1:B:100:VAL:HA  | 6                   | 0.26     | 0.11                | 0.24       |
| (1,1262) | 1:B:103:LYS:HG2  | 1:B:103:LYS:H   | 6                   | 0.26     | 0.13                | 0.22       |
| (1,1262) | 1:B:103:LYS:HG3  | 1:B:103:LYS:H   | 6                   | 0.26     | 0.13                | 0.22       |
| (1,280)  | 1:A:92:LYS:H     | 1:A:100:VAL:HA  | 6                   | 0.26     | 0.11                | 0.24       |
| (1,395)  | 1:A:103:LYS:HG2  | 1:A:103:LYS:H   | 6                   | 0.26     | 0.13                | 0.22       |
| (1,395)  | 1:A:103:LYS:HG3  | 1:A:103:LYS:H   | 6                   | 0.26     | 0.13                | 0.22       |
| (1,1442) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA  | 6                   | 0.23     | 0.06                | 0.22       |
| (1,1443) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA  | 6                   | 0.23     | 0.06                | 0.22       |
| (1,575)  | 1:A:119:HIS:HB3  | 1:A:119:HIS:HA  | 6                   | 0.23     | 0.06                | 0.22       |
| (1,576)  | 1:A:119:HIS:HB3  | 1:A:119:HIS:HA  | 6                   | 0.23     | 0.06                | 0.22       |
| (1,379)  | 1:A:101:HIS:HB2  | 1:A:101:HIS:H   | 6                   | 0.22     | 0.08                | 0.19       |
| (1,1246) | 1:B:101:HIS:HB2  | 1:B:101:HIS:H   | 6                   | 0.22     | 0.08                | 0.19       |
| (1,1281) | 1:B:105:GLU:HG2  | 1:B:105:GLU:H   | 6                   | 0.22     | 0.07                | 0.24       |
| (1,1281) | 1:B:105:GLU:HG3  | 1:B:105:GLU:H   | 6                   | 0.22     | 0.07                | 0.24       |
| (1,746)  | 1:A:136:SER:H    | 1:A:135:SER:H   | 6                   | 0.2      | 0.03                | 0.2        |
| (1,1613) | 1:B:136:SER:H    | 1:B:135:SER:H   | 6                   | 0.2      | 0.03                | 0.2        |
| (1,130)  | 1:A:78:ASN:HB2   | 1:A:79:LEU:H    | 6                   | 0.18     | 0.07                | 0.16       |
| (1,997)  | 1:B:78:ASN:HB2   | 1:B:79:LEU:H    | 6                   | 0.18     | 0.07                | 0.16       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,534)  | 1:A:116:ARG:H    | 1:A:104:HIS:H   | 6                   | 0.18     | 0.1                 | 0.14       |
| (1,535)  | 1:A:116:ARG:H    | 1:A:104:HIS:H   | 6                   | 0.18     | 0.1                 | 0.14       |
| (1,1401) | 1:B:116:ARG:H    | 1:B:104:HIS:H   | 6                   | 0.18     | 0.1                 | 0.14       |
| (1,1402) | 1:B:116:ARG:H    | 1:B:104:HIS:H   | 6                   | 0.18     | 0.1                 | 0.14       |
| (1,1294) | 1:B:107:ARG:HB3  | 1:B:107:ARG:H   | 6                   | 0.17     | 0.04                | 0.16       |
| (1,833)  | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 6                   | 0.12     | 0.01                | 0.12       |
| (1,834)  | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1700) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA  | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1701) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA  | 6                   | 0.12     | 0.01                | 0.12       |
| (1,36)   | 1:A:74:ARG:H     | 1:A:73:ASP:HB2  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,36)   | 1:A:74:ARG:H     | 1:A:73:ASP:HB3  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB2  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB3  | 6                   | 0.11     | 0.0                 | 0.11       |
| (1,618)  | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD1 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,618)  | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD2 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,618)  | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD1 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,618)  | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD2 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,618)  | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD1 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,618)  | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD2 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD1 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD2 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD1 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD2 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD1 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD2 | 5                   | 1.67     | 0.78                | 1.71       |
| (1,483)  | 1:A:113:PHE:HE1  | 1:A:107:ARG:HA  | 5                   | 1.55     | 0.11                | 1.58       |
| (1,483)  | 1:A:113:PHE:HE2  | 1:A:107:ARG:HA  | 5                   | 1.55     | 0.11                | 1.58       |
| (1,1350) | 1:B:113:PHE:HE1  | 1:B:107:ARG:HA  | 5                   | 1.55     | 0.11                | 1.58       |
| (1,1350) | 1:B:113:PHE:HE2  | 1:B:107:ARG:HA  | 5                   | 1.55     | 0.11                | 1.58       |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD1 | 5                   | 1.39     | 0.89                | 1.33       |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD2 | 5                   | 1.39     | 0.89                | 1.33       |
| (1,643)  | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD1 | 5                   | 1.39     | 0.89                | 1.33       |
| (1,643)  | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD2 | 5                   | 1.39     | 0.89                | 1.33       |
| (1,1311) | 1:B:108:GLN:HA   | 1:B:113:PHE:HE1 | 5                   | 1.37     | 0.15                | 1.34       |
| (1,1311) | 1:B:108:GLN:HA   | 1:B:113:PHE:HE2 | 5                   | 1.37     | 0.15                | 1.34       |
| (1,444)  | 1:A:108:GLN:HA   | 1:A:113:PHE:HE1 | 5                   | 1.37     | 0.15                | 1.34       |
| (1,444)  | 1:A:108:GLN:HA   | 1:A:113:PHE:HE2 | 5                   | 1.37     | 0.15                | 1.34       |
| (1,258)  | 1:A:89:LEU:HD11  | 1:A:102:GLY:HA2 | 5                   | 1.31     | 0.2                 | 1.29       |
| (1,258)  | 1:A:89:LEU:HD12  | 1:A:102:GLY:HA2 | 5                   | 1.31     | 0.2                 | 1.29       |
| (1,258)  | 1:A:89:LEU:HD13  | 1:A:102:GLY:HA2 | 5                   | 1.31     | 0.2                 | 1.29       |
| (1,1125) | 1:B:89:LEU:HD11  | 1:B:102:GLY:HA2 | 5                   | 1.31     | 0.2                 | 1.29       |
| (1,1125) | 1:B:89:LEU:HD12  | 1:B:102:GLY:HA2 | 5                   | 1.31     | 0.2                 | 1.29       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1125) | 1:B:89:LEU:HD13 | 1:B:102:GLY:HA2 | 5                   | 1.31     | 0.2                 | 1.29       |
| (1,342)  | 1:A:98:ILE:HD11 | 1:A:122:TYR:HD1 | 5                   | 1.2      | 0.15                | 1.19       |
| (1,342)  | 1:A:98:ILE:HD11 | 1:A:122:TYR:HD2 | 5                   | 1.2      | 0.15                | 1.19       |
| (1,342)  | 1:A:98:ILE:HD12 | 1:A:122:TYR:HD1 | 5                   | 1.2      | 0.15                | 1.19       |
| (1,342)  | 1:A:98:ILE:HD12 | 1:A:122:TYR:HD2 | 5                   | 1.2      | 0.15                | 1.19       |
| (1,342)  | 1:A:98:ILE:HD13 | 1:A:122:TYR:HD1 | 5                   | 1.2      | 0.15                | 1.19       |
| (1,342)  | 1:A:98:ILE:HD13 | 1:A:122:TYR:HD2 | 5                   | 1.2      | 0.15                | 1.19       |
| (1,1209) | 1:B:98:ILE:HD11 | 1:B:122:TYR:HD1 | 5                   | 1.19     | 0.16                | 1.19       |
| (1,1209) | 1:B:98:ILE:HD11 | 1:B:122:TYR:HD2 | 5                   | 1.19     | 0.16                | 1.19       |
| (1,1209) | 1:B:98:ILE:HD12 | 1:B:122:TYR:HD1 | 5                   | 1.19     | 0.16                | 1.19       |
| (1,1209) | 1:B:98:ILE:HD12 | 1:B:122:TYR:HD2 | 5                   | 1.19     | 0.16                | 1.19       |
| (1,1209) | 1:B:98:ILE:HD13 | 1:B:122:TYR:HD1 | 5                   | 1.19     | 0.16                | 1.19       |
| (1,1209) | 1:B:98:ILE:HD13 | 1:B:122:TYR:HD2 | 5                   | 1.19     | 0.16                | 1.19       |
| (1,595)  | 1:A:122:TYR:HD1 | 1:A:122:TYR:H   | 5                   | 1.06     | 0.48                | 1.21       |
| (1,595)  | 1:A:122:TYR:HD2 | 1:A:122:TYR:H   | 5                   | 1.06     | 0.48                | 1.21       |
| (1,1462) | 1:B:122:TYR:HD1 | 1:B:122:TYR:H   | 5                   | 1.06     | 0.48                | 1.21       |
| (1,1462) | 1:B:122:TYR:HD2 | 1:B:122:TYR:H   | 5                   | 1.06     | 0.48                | 1.21       |
| (1,126)  | 1:A:78:ASN:H    | 1:A:78:ASN:HD22 | 5                   | 1.05     | 0.15                | 0.95       |
| (1,993)  | 1:B:78:ASN:H    | 1:B:78:ASN:HD22 | 5                   | 1.05     | 0.15                | 0.95       |
| (1,6)    | 1:A:67:GLU:H    | 1:A:67:GLU:HG2  | 5                   | 1.03     | 0.07                | 0.99       |
| (1,6)    | 1:A:67:GLU:H    | 1:A:67:GLU:HG3  | 5                   | 1.03     | 0.07                | 0.99       |
| (1,873)  | 1:B:67:GLU:H    | 1:B:67:GLU:HG2  | 5                   | 1.03     | 0.07                | 0.99       |
| (1,873)  | 1:B:67:GLU:H    | 1:B:67:GLU:HG3  | 5                   | 1.03     | 0.07                | 0.99       |
| (1,150)  | 1:A:81:VAL:HG11 | 1:A:79:LEU:HB2  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,150)  | 1:A:81:VAL:HG11 | 1:A:79:LEU:HB3  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,150)  | 1:A:81:VAL:HG12 | 1:A:79:LEU:HB2  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,150)  | 1:A:81:VAL:HG12 | 1:A:79:LEU:HB3  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,150)  | 1:A:81:VAL:HG13 | 1:A:79:LEU:HB2  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,150)  | 1:A:81:VAL:HG13 | 1:A:79:LEU:HB3  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,1017) | 1:B:81:VAL:HG11 | 1:B:79:LEU:HB2  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,1017) | 1:B:81:VAL:HG11 | 1:B:79:LEU:HB3  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,1017) | 1:B:81:VAL:HG12 | 1:B:79:LEU:HB2  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,1017) | 1:B:81:VAL:HG12 | 1:B:79:LEU:HB3  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,1017) | 1:B:81:VAL:HG13 | 1:B:79:LEU:HB2  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,1017) | 1:B:81:VAL:HG13 | 1:B:79:LEU:HB3  | 5                   | 0.89     | 0.35                | 1.04       |
| (1,1270) | 1:B:104:HIS:HA  | 1:B:104:HIS:HD2 | 5                   | 0.89     | 0.04                | 0.89       |
| (1,403)  | 1:A:104:HIS:HA  | 1:A:104:HIS:HD2 | 5                   | 0.87     | 0.05                | 0.87       |
| (1,954)  | 1:B:77:VAL:HG21 | 1:B:75:PHE:HD1  | 5                   | 0.87     | 0.38                | 1.0        |
| (1,954)  | 1:B:77:VAL:HG21 | 1:B:75:PHE:HD2  | 5                   | 0.87     | 0.38                | 1.0        |
| (1,954)  | 1:B:77:VAL:HG22 | 1:B:75:PHE:HD1  | 5                   | 0.87     | 0.38                | 1.0        |
| (1,954)  | 1:B:77:VAL:HG22 | 1:B:75:PHE:HD2  | 5                   | 0.87     | 0.38                | 1.0        |
| (1,954)  | 1:B:77:VAL:HG23 | 1:B:75:PHE:HD1  | 5                   | 0.87     | 0.38                | 1.0        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,954)  | 1:B:77:VAL:HG23 | 1:B:75:PHE:HD2  | 5                   | 0.87     | 0.38                | 1.0        |
| (1,87)   | 1:A:77:VAL:HG21 | 1:A:75:PHE:HD1  | 5                   | 0.87     | 0.38                | 0.99       |
| (1,87)   | 1:A:77:VAL:HG21 | 1:A:75:PHE:HD2  | 5                   | 0.87     | 0.38                | 0.99       |
| (1,87)   | 1:A:77:VAL:HG22 | 1:A:75:PHE:HD1  | 5                   | 0.87     | 0.38                | 0.99       |
| (1,87)   | 1:A:77:VAL:HG22 | 1:A:75:PHE:HD2  | 5                   | 0.87     | 0.38                | 0.99       |
| (1,87)   | 1:A:77:VAL:HG23 | 1:A:75:PHE:HD1  | 5                   | 0.87     | 0.38                | 0.99       |
| (1,87)   | 1:A:77:VAL:HG23 | 1:A:75:PHE:HD2  | 5                   | 0.87     | 0.38                | 0.99       |
| (1,185)  | 1:A:83:HIS:HB3  | 1:A:104:HIS:HB2 | 5                   | 0.85     | 0.75                | 0.48       |
| (1,1052) | 1:B:83:HIS:HB3  | 1:B:104:HIS:HB2 | 5                   | 0.85     | 0.75                | 0.48       |
| (1,1729) | 1:B:150:LYS:HG2 | 1:B:151:GLN:H   | 5                   | 0.85     | 0.13                | 0.91       |
| (1,1729) | 1:B:150:LYS:HG3 | 1:B:151:GLN:H   | 5                   | 0.85     | 0.13                | 0.91       |
| (1,862)  | 1:A:150:LYS:HG2 | 1:A:151:GLN:H   | 5                   | 0.85     | 0.13                | 0.9        |
| (1,862)  | 1:A:150:LYS:HG3 | 1:A:151:GLN:H   | 5                   | 0.85     | 0.13                | 0.9        |
| (1,604)  | 1:A:123:ARG:HB2 | 1:A:97:VAL:HG11 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,604)  | 1:A:123:ARG:HB2 | 1:A:97:VAL:HG12 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,604)  | 1:A:123:ARG:HB2 | 1:A:97:VAL:HG13 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,604)  | 1:A:123:ARG:HB2 | 1:A:97:VAL:HG21 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,604)  | 1:A:123:ARG:HB2 | 1:A:97:VAL:HG22 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,604)  | 1:A:123:ARG:HB2 | 1:A:97:VAL:HG23 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,1324) | 1:B:111:HIS:H   | 1:B:109:ASP:HB2 | 5                   | 0.8      | 0.44                | 0.97       |
| (1,1324) | 1:B:111:HIS:H   | 1:B:109:ASP:HB3 | 5                   | 0.8      | 0.44                | 0.97       |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG11 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG12 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG13 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG21 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG22 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG23 | 5                   | 0.8      | 0.21                | 0.77       |
| (1,457)  | 1:A:111:HIS:H   | 1:A:109:ASP:HB2 | 5                   | 0.79     | 0.44                | 0.96       |
| (1,457)  | 1:A:111:HIS:H   | 1:A:109:ASP:HB3 | 5                   | 0.79     | 0.44                | 0.96       |
| (1,1467) | 1:B:122:TYR:HA  | 1:B:123:ARG:HB3 | 5                   | 0.79     | 0.28                | 0.91       |
| (1,600)  | 1:A:122:TYR:HA  | 1:A:123:ARG:HB3 | 5                   | 0.79     | 0.28                | 0.9        |
| (1,368)  | 1:A:101:HIS:HB2 | 1:A:92:LYS:HB2  | 5                   | 0.7      | 0.57                | 0.44       |
| (1,368)  | 1:A:101:HIS:HB2 | 1:A:92:LYS:HB3  | 5                   | 0.7      | 0.57                | 0.44       |
| (1,1235) | 1:B:101:HIS:HB2 | 1:B:92:LYS:HB2  | 5                   | 0.7      | 0.57                | 0.44       |
| (1,1235) | 1:B:101:HIS:HB2 | 1:B:92:LYS:HB3  | 5                   | 0.7      | 0.57                | 0.44       |
| (1,243)  | 1:A:89:LEU:HD11 | 1:A:88:GLU:H    | 5                   | 0.66     | 0.13                | 0.61       |
| (1,243)  | 1:A:89:LEU:HD12 | 1:A:88:GLU:H    | 5                   | 0.66     | 0.13                | 0.61       |
| (1,243)  | 1:A:89:LEU:HD13 | 1:A:88:GLU:H    | 5                   | 0.66     | 0.13                | 0.61       |
| (1,1110) | 1:B:89:LEU:HD11 | 1:B:88:GLU:H    | 5                   | 0.66     | 0.13                | 0.61       |
| (1,1110) | 1:B:89:LEU:HD12 | 1:B:88:GLU:H    | 5                   | 0.66     | 0.13                | 0.61       |
| (1,1110) | 1:B:89:LEU:HD13 | 1:B:88:GLU:H    | 5                   | 0.66     | 0.13                | 0.61       |
| (1,1058) | 1:B:84:PHE:HD1  | 1:B:82:LYS:H    | 5                   | 0.57     | 0.42                | 0.37       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1058) | 1:B:84:PHE:HD2   | 1:B:82:LYS:H    | 5                   | 0.57     | 0.42                | 0.37       |
| (1,191)  | 1:A:84:PHE:HD1   | 1:A:82:LYS:H    | 5                   | 0.57     | 0.42                | 0.37       |
| (1,191)  | 1:A:84:PHE:HD2   | 1:A:82:LYS:H    | 5                   | 0.57     | 0.42                | 0.37       |
| (1,1047) | 1:B:83:HIS:HB2   | 1:B:83:HIS:H    | 5                   | 0.53     | 0.17                | 0.57       |
| (1,180)  | 1:A:83:HIS:HB2   | 1:A:83:HIS:H    | 5                   | 0.53     | 0.17                | 0.57       |
| (1,492)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HE1 | 5                   | 0.53     | 0.03                | 0.54       |
| (1,492)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HE2 | 5                   | 0.53     | 0.03                | 0.54       |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE1 | 5                   | 0.53     | 0.03                | 0.54       |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE2 | 5                   | 0.53     | 0.03                | 0.54       |
| (1,451)  | 1:A:109:ASP:H    | 1:A:112:GLY:H   | 5                   | 0.5      | 0.19                | 0.54       |
| (1,1318) | 1:B:109:ASP:H    | 1:B:112:GLY:H   | 5                   | 0.5      | 0.19                | 0.54       |
| (1,63)   | 1:A:76:SER:HB2   | 1:A:77:VAL:H    | 5                   | 0.49     | 0.2                 | 0.46       |
| (1,930)  | 1:B:76:SER:HB2   | 1:B:77:VAL:H    | 5                   | 0.49     | 0.2                 | 0.46       |
| (1,112)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HD1 | 5                   | 0.47     | 0.2                 | 0.45       |
| (1,112)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HD2 | 5                   | 0.47     | 0.2                 | 0.45       |
| (1,112)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HD1 | 5                   | 0.47     | 0.2                 | 0.45       |
| (1,112)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HD2 | 5                   | 0.47     | 0.2                 | 0.45       |
| (1,112)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HD1 | 5                   | 0.47     | 0.2                 | 0.45       |
| (1,112)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HD2 | 5                   | 0.47     | 0.2                 | 0.45       |
| (1,979)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HD1 | 5                   | 0.47     | 0.21                | 0.45       |
| (1,979)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HD2 | 5                   | 0.47     | 0.21                | 0.45       |
| (1,979)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HD1 | 5                   | 0.47     | 0.21                | 0.45       |
| (1,979)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HD2 | 5                   | 0.47     | 0.21                | 0.45       |
| (1,979)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HD1 | 5                   | 0.47     | 0.21                | 0.45       |
| (1,979)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HD2 | 5                   | 0.47     | 0.21                | 0.45       |
| (1,163)  | 1:A:81:VAL:HG21  | 1:A:83:HIS:H    | 5                   | 0.46     | 0.26                | 0.45       |
| (1,163)  | 1:A:81:VAL:HG22  | 1:A:83:HIS:H    | 5                   | 0.46     | 0.26                | 0.45       |
| (1,163)  | 1:A:81:VAL:HG23  | 1:A:83:HIS:H    | 5                   | 0.46     | 0.26                | 0.45       |
| (1,1030) | 1:B:81:VAL:HG21  | 1:B:83:HIS:H    | 5                   | 0.46     | 0.26                | 0.45       |
| (1,1030) | 1:B:81:VAL:HG22  | 1:B:83:HIS:H    | 5                   | 0.46     | 0.26                | 0.45       |
| (1,1030) | 1:B:81:VAL:HG23  | 1:B:83:HIS:H    | 5                   | 0.46     | 0.26                | 0.45       |
| (1,488)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB2 | 5                   | 0.46     | 0.03                | 0.46       |
| (1,1355) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB2 | 5                   | 0.46     | 0.03                | 0.46       |
| (1,62)   | 1:A:76:SER:HB3   | 1:A:76:SER:H    | 5                   | 0.44     | 0.1                 | 0.4        |
| (1,929)  | 1:B:76:SER:HB3   | 1:B:76:SER:H    | 5                   | 0.44     | 0.1                 | 0.4        |
| (1,1733) | 1:B:152:VAL:H    | 1:B:151:GLN:H   | 5                   | 0.4      | 0.24                | 0.38       |
| (1,866)  | 1:A:152:VAL:H    | 1:A:151:GLN:H   | 5                   | 0.4      | 0.23                | 0.38       |
| (1,782)  | 1:A:142:VAL:HG11 | 1:A:142:VAL:H   | 5                   | 0.39     | 0.1                 | 0.41       |
| (1,782)  | 1:A:142:VAL:HG12 | 1:A:142:VAL:H   | 5                   | 0.39     | 0.1                 | 0.41       |
| (1,782)  | 1:A:142:VAL:HG13 | 1:A:142:VAL:H   | 5                   | 0.39     | 0.1                 | 0.41       |
| (1,782)  | 1:A:142:VAL:HG21 | 1:A:142:VAL:H   | 5                   | 0.39     | 0.1                 | 0.41       |
| (1,782)  | 1:A:142:VAL:HG22 | 1:A:142:VAL:H   | 5                   | 0.39     | 0.1                 | 0.41       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,782)  | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 5                   | 0.39     | 0.1                 | 0.41       |
| (1,783)  | 1:A:142:VAL:HG11 | 1:A:142:VAL:H    | 5                   | 0.39     | 0.1                 | 0.41       |
| (1,783)  | 1:A:142:VAL:HG12 | 1:A:142:VAL:H    | 5                   | 0.39     | 0.1                 | 0.41       |
| (1,783)  | 1:A:142:VAL:HG13 | 1:A:142:VAL:H    | 5                   | 0.39     | 0.1                 | 0.41       |
| (1,783)  | 1:A:142:VAL:HG21 | 1:A:142:VAL:H    | 5                   | 0.39     | 0.1                 | 0.41       |
| (1,783)  | 1:A:142:VAL:HG22 | 1:A:142:VAL:H    | 5                   | 0.39     | 0.1                 | 0.41       |
| (1,783)  | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 5                   | 0.39     | 0.1                 | 0.41       |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG21  | 5                   | 0.38     | 0.34                | 0.19       |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG22  | 5                   | 0.38     | 0.34                | 0.19       |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG23  | 5                   | 0.38     | 0.34                | 0.19       |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG21  | 5                   | 0.38     | 0.34                | 0.19       |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG22  | 5                   | 0.38     | 0.34                | 0.19       |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG23  | 5                   | 0.38     | 0.34                | 0.19       |
| (1,589)  | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG21  | 5                   | 0.38     | 0.34                | 0.2        |
| (1,589)  | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG22  | 5                   | 0.38     | 0.34                | 0.2        |
| (1,589)  | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG23  | 5                   | 0.38     | 0.34                | 0.2        |
| (1,589)  | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG21  | 5                   | 0.38     | 0.34                | 0.2        |
| (1,589)  | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG22  | 5                   | 0.38     | 0.34                | 0.2        |
| (1,589)  | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG23  | 5                   | 0.38     | 0.34                | 0.2        |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD11 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD12 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD13 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD21 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD22 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD23 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD11 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD12 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD13 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD21 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD22 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD23 | 5                   | 0.38     | 0.16                | 0.48       |
| (1,216)  | 1:A:85:SER:HB2   | 1:A:89:LEU:H     | 5                   | 0.33     | 0.14                | 0.27       |
| (1,1083) | 1:B:85:SER:HB2   | 1:B:89:LEU:H     | 5                   | 0.33     | 0.14                | 0.27       |
| (1,1225) | 1:B:100:VAL:HG11 | 1:B:92:LYS:H     | 5                   | 0.33     | 0.24                | 0.16       |
| (1,1225) | 1:B:100:VAL:HG12 | 1:B:92:LYS:H     | 5                   | 0.33     | 0.24                | 0.16       |
| (1,1225) | 1:B:100:VAL:HG13 | 1:B:92:LYS:H     | 5                   | 0.33     | 0.24                | 0.16       |
| (1,259)  | 1:A:89:LEU:HD11  | 1:A:103:LYS:H    | 5                   | 0.32     | 0.19                | 0.29       |
| (1,259)  | 1:A:89:LEU:HD12  | 1:A:103:LYS:H    | 5                   | 0.32     | 0.19                | 0.29       |
| (1,259)  | 1:A:89:LEU:HD13  | 1:A:103:LYS:H    | 5                   | 0.32     | 0.19                | 0.29       |
| (1,358)  | 1:A:100:VAL:HG11 | 1:A:92:LYS:H     | 5                   | 0.32     | 0.24                | 0.16       |
| (1,358)  | 1:A:100:VAL:HG12 | 1:A:92:LYS:H     | 5                   | 0.32     | 0.24                | 0.16       |
| (1,358)  | 1:A:100:VAL:HG13 | 1:A:92:LYS:H     | 5                   | 0.32     | 0.24                | 0.16       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,447)  | 1:A:109:ASP:H   | 1:A:109:ASP:HB2 | 5                   | 0.32     | 0.16                | 0.27       |
| (1,447)  | 1:A:109:ASP:H   | 1:A:109:ASP:HB3 | 5                   | 0.32     | 0.16                | 0.27       |
| (1,1126) | 1:B:89:LEU:HD11 | 1:B:103:LYS:H   | 5                   | 0.32     | 0.19                | 0.29       |
| (1,1126) | 1:B:89:LEU:HD12 | 1:B:103:LYS:H   | 5                   | 0.32     | 0.19                | 0.29       |
| (1,1126) | 1:B:89:LEU:HD13 | 1:B:103:LYS:H   | 5                   | 0.32     | 0.19                | 0.29       |
| (1,1314) | 1:B:109:ASP:H   | 1:B:109:ASP:HB2 | 5                   | 0.32     | 0.16                | 0.26       |
| (1,1314) | 1:B:109:ASP:H   | 1:B:109:ASP:HB3 | 5                   | 0.32     | 0.16                | 0.26       |
| (1,215)  | 1:A:85:SER:HB3  | 1:A:89:LEU:H    | 5                   | 0.29     | 0.13                | 0.21       |
| (1,1082) | 1:B:85:SER:HB3  | 1:B:89:LEU:H    | 5                   | 0.29     | 0.13                | 0.21       |
| (1,812)  | 1:A:145:VAL:HB  | 1:A:135:SER:HA  | 5                   | 0.29     | 0.11                | 0.27       |
| (1,1679) | 1:B:145:VAL:HB  | 1:B:135:SER:HA  | 5                   | 0.29     | 0.1                 | 0.27       |
| (1,1455) | 1:B:122:TYR:HB2 | 1:B:98:ILE:HD11 | 5                   | 0.28     | 0.09                | 0.26       |
| (1,1455) | 1:B:122:TYR:HB2 | 1:B:98:ILE:HD12 | 5                   | 0.28     | 0.09                | 0.26       |
| (1,1455) | 1:B:122:TYR:HB2 | 1:B:98:ILE:HD13 | 5                   | 0.28     | 0.09                | 0.26       |
| (1,1455) | 1:B:122:TYR:HB3 | 1:B:98:ILE:HD11 | 5                   | 0.28     | 0.09                | 0.26       |
| (1,1455) | 1:B:122:TYR:HB3 | 1:B:98:ILE:HD12 | 5                   | 0.28     | 0.09                | 0.26       |
| (1,1455) | 1:B:122:TYR:HB3 | 1:B:98:ILE:HD13 | 5                   | 0.28     | 0.09                | 0.26       |
| (1,706)  | 1:A:132:THR:H   | 1:A:133:ILE:H   | 5                   | 0.28     | 0.07                | 0.28       |
| (1,708)  | 1:A:132:THR:H   | 1:A:133:ILE:H   | 5                   | 0.28     | 0.07                | 0.28       |
| (1,1573) | 1:B:132:THR:H   | 1:B:133:ILE:H   | 5                   | 0.28     | 0.07                | 0.28       |
| (1,1575) | 1:B:132:THR:H   | 1:B:133:ILE:H   | 5                   | 0.28     | 0.07                | 0.28       |
| (1,740)  | 1:A:135:SER:HA  | 1:A:145:VAL:HA  | 5                   | 0.27     | 0.07                | 0.31       |
| (1,742)  | 1:A:135:SER:HA  | 1:A:145:VAL:HA  | 5                   | 0.27     | 0.07                | 0.31       |
| (1,1607) | 1:B:135:SER:HA  | 1:B:145:VAL:HA  | 5                   | 0.27     | 0.07                | 0.31       |
| (1,1609) | 1:B:135:SER:HA  | 1:B:145:VAL:HA  | 5                   | 0.27     | 0.07                | 0.31       |
| (1,588)  | 1:A:122:TYR:HB2 | 1:A:98:ILE:HD11 | 5                   | 0.24     | 0.04                | 0.25       |
| (1,588)  | 1:A:122:TYR:HB2 | 1:A:98:ILE:HD12 | 5                   | 0.24     | 0.04                | 0.25       |
| (1,588)  | 1:A:122:TYR:HB2 | 1:A:98:ILE:HD13 | 5                   | 0.24     | 0.04                | 0.25       |
| (1,588)  | 1:A:122:TYR:HB3 | 1:A:98:ILE:HD11 | 5                   | 0.24     | 0.04                | 0.25       |
| (1,588)  | 1:A:122:TYR:HB3 | 1:A:98:ILE:HD12 | 5                   | 0.24     | 0.04                | 0.25       |
| (1,588)  | 1:A:122:TYR:HB3 | 1:A:98:ILE:HD13 | 5                   | 0.24     | 0.04                | 0.25       |
| (1,414)  | 1:A:105:GLU:HG2 | 1:A:105:GLU:H   | 5                   | 0.24     | 0.06                | 0.25       |
| (1,414)  | 1:A:105:GLU:HG3 | 1:A:105:GLU:H   | 5                   | 0.24     | 0.06                | 0.25       |
| (1,1282) | 1:B:105:GLU:HA  | 1:B:106:GLU:H   | 5                   | 0.21     | 0.07                | 0.2        |
| (1,415)  | 1:A:105:GLU:HA  | 1:A:106:GLU:H   | 5                   | 0.2      | 0.06                | 0.19       |
| (1,988)  | 1:B:78:ASN:HA   | 1:B:78:ASN:HB2  | 5                   | 0.19     | 0.01                | 0.19       |
| (1,121)  | 1:A:78:ASN:HA   | 1:A:78:ASN:HB2  | 5                   | 0.19     | 0.01                | 0.19       |
| (1,478)  | 1:A:112:GLY:HA2 | 1:A:112:GLY:H   | 5                   | 0.18     | 0.02                | 0.19       |
| (1,1345) | 1:B:112:GLY:HA2 | 1:B:112:GLY:H   | 5                   | 0.18     | 0.02                | 0.19       |
| (1,427)  | 1:A:107:ARG:HB3 | 1:A:107:ARG:H   | 5                   | 0.18     | 0.04                | 0.18       |
| (1,803)  | 1:A:144:THR:H   | 1:A:145:VAL:H   | 5                   | 0.18     | 0.06                | 0.16       |
| (1,808)  | 1:A:144:THR:H   | 1:A:145:VAL:H   | 5                   | 0.18     | 0.06                | 0.16       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1670) | 1:B:144:THR:H   | 1:B:145:VAL:H    | 5                   | 0.18     | 0.05                | 0.16       |
| (1,1675) | 1:B:144:THR:H   | 1:B:145:VAL:H    | 5                   | 0.18     | 0.05                | 0.16       |
| (1,856)  | 1:A:150:LYS:H   | 1:A:149:ARG:H    | 5                   | 0.15     | 0.03                | 0.16       |
| (1,1723) | 1:B:150:LYS:H   | 1:B:149:ARG:H    | 5                   | 0.15     | 0.02                | 0.16       |
| (1,7)    | 1:A:68:MET:HA   | 1:A:68:MET:HG2   | 5                   | 0.14     | 0.01                | 0.13       |
| (1,7)    | 1:A:68:MET:HA   | 1:A:68:MET:HG3   | 5                   | 0.14     | 0.01                | 0.13       |
| (1,874)  | 1:B:68:MET:HA   | 1:B:68:MET:HG2   | 5                   | 0.14     | 0.01                | 0.13       |
| (1,874)  | 1:B:68:MET:HA   | 1:B:68:MET:HG3   | 5                   | 0.14     | 0.01                | 0.13       |
| (1,619)  | 1:A:124:ILE:HA  | 1:A:122:TYR:HD1  | 4                   | 1.73     | 0.65                | 1.74       |
| (1,619)  | 1:A:124:ILE:HA  | 1:A:122:TYR:HD2  | 4                   | 1.73     | 0.65                | 1.74       |
| (1,1486) | 1:B:124:ILE:HA  | 1:B:122:TYR:HD1  | 4                   | 1.73     | 0.65                | 1.74       |
| (1,1486) | 1:B:124:ILE:HA  | 1:B:122:TYR:HD2  | 4                   | 1.73     | 0.65                | 1.74       |
| (1,39)   | 1:A:74:ARG:HG2  | 1:A:73:ASP:H     | 4                   | 1.43     | 0.25                | 1.38       |
| (1,39)   | 1:A:74:ARG:HG3  | 1:A:73:ASP:H     | 4                   | 1.43     | 0.25                | 1.38       |
| (1,906)  | 1:B:74:ARG:HG2  | 1:B:73:ASP:H     | 4                   | 1.43     | 0.25                | 1.38       |
| (1,906)  | 1:B:74:ARG:HG3  | 1:B:73:ASP:H     | 4                   | 1.43     | 0.25                | 1.38       |
| (1,190)  | 1:A:84:PHE:HE1  | 1:A:82:LYS:H     | 4                   | 1.17     | 0.26                | 1.26       |
| (1,190)  | 1:A:84:PHE:HE2  | 1:A:82:LYS:H     | 4                   | 1.17     | 0.26                | 1.26       |
| (1,1057) | 1:B:84:PHE:HE1  | 1:B:82:LYS:H     | 4                   | 1.17     | 0.26                | 1.25       |
| (1,1057) | 1:B:84:PHE:HE2  | 1:B:82:LYS:H     | 4                   | 1.17     | 0.26                | 1.25       |
| (1,194)  | 1:A:84:PHE:HD1  | 1:A:83:HIS:H     | 4                   | 1.12     | 0.36                | 1.12       |
| (1,194)  | 1:A:84:PHE:HD2  | 1:A:83:HIS:H     | 4                   | 1.12     | 0.36                | 1.12       |
| (1,1061) | 1:B:84:PHE:HD1  | 1:B:83:HIS:H     | 4                   | 1.12     | 0.36                | 1.12       |
| (1,1061) | 1:B:84:PHE:HD2  | 1:B:83:HIS:H     | 4                   | 1.12     | 0.36                | 1.12       |
| (1,76)   | 1:A:76:SER:HB3  | 1:A:146:ASP:HA   | 4                   | 1.07     | 0.05                | 1.08       |
| (1,943)  | 1:B:76:SER:HB3  | 1:B:146:ASP:HA   | 4                   | 1.07     | 0.05                | 1.08       |
| (1,69)   | 1:A:76:SER:HB3  | 1:A:146:ASP:HA   | 4                   | 1.02     | 0.05                | 1.02       |
| (1,936)  | 1:B:76:SER:HB3  | 1:B:146:ASP:HA   | 4                   | 1.02     | 0.05                | 1.02       |
| (1,53)   | 1:A:75:PHE:HE1  | 1:A:133:ILE:HD11 | 4                   | 0.97     | 0.36                | 0.93       |
| (1,53)   | 1:A:75:PHE:HE1  | 1:A:133:ILE:HD12 | 4                   | 0.97     | 0.36                | 0.93       |
| (1,53)   | 1:A:75:PHE:HE1  | 1:A:133:ILE:HD13 | 4                   | 0.97     | 0.36                | 0.93       |
| (1,53)   | 1:A:75:PHE:HE2  | 1:A:133:ILE:HD11 | 4                   | 0.97     | 0.36                | 0.93       |
| (1,53)   | 1:A:75:PHE:HE2  | 1:A:133:ILE:HD12 | 4                   | 0.97     | 0.36                | 0.93       |
| (1,53)   | 1:A:75:PHE:HE2  | 1:A:133:ILE:HD13 | 4                   | 0.97     | 0.36                | 0.93       |
| (1,920)  | 1:B:75:PHE:HE1  | 1:B:133:ILE:HD11 | 4                   | 0.96     | 0.36                | 0.94       |
| (1,920)  | 1:B:75:PHE:HE1  | 1:B:133:ILE:HD12 | 4                   | 0.96     | 0.36                | 0.94       |
| (1,920)  | 1:B:75:PHE:HE1  | 1:B:133:ILE:HD13 | 4                   | 0.96     | 0.36                | 0.94       |
| (1,920)  | 1:B:75:PHE:HE2  | 1:B:133:ILE:HD11 | 4                   | 0.96     | 0.36                | 0.94       |
| (1,920)  | 1:B:75:PHE:HE2  | 1:B:133:ILE:HD12 | 4                   | 0.96     | 0.36                | 0.94       |
| (1,920)  | 1:B:75:PHE:HE2  | 1:B:133:ILE:HD13 | 4                   | 0.96     | 0.36                | 0.94       |
| (1,1740) | 1:A:113:PHE:HD1 | 1:B:121:LYS:H    | 4                   | 0.84     | 0.22                | 0.8        |
| (1,1740) | 1:A:113:PHE:HD2 | 1:B:121:LYS:H    | 4                   | 0.84     | 0.22                | 0.8        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,238)  | 1:A:89:LEU:HD11  | 1:A:85:SER:H     | 4                   | 0.82     | 0.5                 | 0.74       |
| (1,238)  | 1:A:89:LEU:HD12  | 1:A:85:SER:H     | 4                   | 0.82     | 0.5                 | 0.74       |
| (1,238)  | 1:A:89:LEU:HD13  | 1:A:85:SER:H     | 4                   | 0.82     | 0.5                 | 0.74       |
| (1,1105) | 1:B:89:LEU:HD11  | 1:B:85:SER:H     | 4                   | 0.82     | 0.5                 | 0.74       |
| (1,1105) | 1:B:89:LEU:HD12  | 1:B:85:SER:H     | 4                   | 0.82     | 0.5                 | 0.74       |
| (1,1105) | 1:B:89:LEU:HD13  | 1:B:85:SER:H     | 4                   | 0.82     | 0.5                 | 0.74       |
| (1,551)  | 1:A:118:PHE:HD1  | 1:A:103:LYS:HA   | 4                   | 0.79     | 0.43                | 0.9        |
| (1,551)  | 1:A:118:PHE:HD2  | 1:A:103:LYS:HA   | 4                   | 0.79     | 0.43                | 0.9        |
| (1,1418) | 1:B:118:PHE:HD1  | 1:B:103:LYS:HA   | 4                   | 0.79     | 0.43                | 0.9        |
| (1,1418) | 1:B:118:PHE:HD2  | 1:B:103:LYS:HA   | 4                   | 0.79     | 0.43                | 0.9        |
| (1,41)   | 1:A:74:ARG:HG2   | 1:A:74:ARG:H     | 4                   | 0.73     | 0.03                | 0.72       |
| (1,41)   | 1:A:74:ARG:HG3   | 1:A:74:ARG:H     | 4                   | 0.73     | 0.03                | 0.72       |
| (1,908)  | 1:B:74:ARG:HG2   | 1:B:74:ARG:H     | 4                   | 0.73     | 0.03                | 0.72       |
| (1,908)  | 1:B:74:ARG:HG3   | 1:B:74:ARG:H     | 4                   | 0.73     | 0.03                | 0.72       |
| (1,1736) | 1:A:111:HIS:HB2  | 1:B:122:TYR:HE1  | 4                   | 0.71     | 0.32                | 0.68       |
| (1,1736) | 1:A:111:HIS:HB2  | 1:B:122:TYR:HE2  | 4                   | 0.71     | 0.32                | 0.68       |
| (1,1595) | 1:B:133:ILE:HG12 | 1:B:147:GLY:HA2  | 4                   | 0.66     | 0.41                | 0.64       |
| (1,1595) | 1:B:133:ILE:HG13 | 1:B:147:GLY:HA2  | 4                   | 0.66     | 0.41                | 0.64       |
| (1,728)  | 1:A:133:ILE:HG12 | 1:A:147:GLY:HA2  | 4                   | 0.66     | 0.4                 | 0.64       |
| (1,728)  | 1:A:133:ILE:HG13 | 1:A:147:GLY:HA2  | 4                   | 0.66     | 0.4                 | 0.64       |
| (1,498)  | 1:A:113:PHE:HB2  | 1:A:113:PHE:H    | 4                   | 0.65     | 0.13                | 0.68       |
| (1,1365) | 1:B:113:PHE:HB2  | 1:B:113:PHE:H    | 4                   | 0.65     | 0.13                | 0.68       |
| (1,26)   | 1:A:71:GLU:H     | 1:A:76:SER:H     | 4                   | 0.64     | 0.49                | 0.48       |
| (1,893)  | 1:B:71:GLU:H     | 1:B:76:SER:H     | 4                   | 0.64     | 0.49                | 0.48       |
| (1,1768) | 1:A:122:TYR:HA   | 1:B:112:GLY:H    | 4                   | 0.62     | 0.18                | 0.66       |
| (1,181)  | 1:A:83:HIS:HB2   | 1:A:84:PHE:HB2   | 4                   | 0.6      | 0.19                | 0.66       |
| (1,181)  | 1:A:83:HIS:HB2   | 1:A:84:PHE:HB3   | 4                   | 0.6      | 0.19                | 0.66       |
| (1,1048) | 1:B:83:HIS:HB2   | 1:B:84:PHE:HB2   | 4                   | 0.6      | 0.19                | 0.65       |
| (1,1048) | 1:B:83:HIS:HB2   | 1:B:84:PHE:HB3   | 4                   | 0.6      | 0.19                | 0.65       |
| (1,559)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HD1  | 4                   | 0.58     | 0.29                | 0.68       |
| (1,559)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HD2  | 4                   | 0.58     | 0.29                | 0.68       |
| (1,1426) | 1:B:118:PHE:HA   | 1:B:118:PHE:HD1  | 4                   | 0.58     | 0.29                | 0.68       |
| (1,1426) | 1:B:118:PHE:HA   | 1:B:118:PHE:HD2  | 4                   | 0.58     | 0.29                | 0.68       |
| (1,65)   | 1:A:76:SER:HB2   | 1:A:144:THR:HG21 | 4                   | 0.58     | 0.23                | 0.6        |
| (1,65)   | 1:A:76:SER:HB2   | 1:A:144:THR:HG22 | 4                   | 0.58     | 0.23                | 0.6        |
| (1,65)   | 1:A:76:SER:HB2   | 1:A:144:THR:HG23 | 4                   | 0.58     | 0.23                | 0.6        |
| (1,932)  | 1:B:76:SER:HB2   | 1:B:144:THR:HG21 | 4                   | 0.58     | 0.23                | 0.6        |
| (1,932)  | 1:B:76:SER:HB2   | 1:B:144:THR:HG22 | 4                   | 0.58     | 0.23                | 0.6        |
| (1,932)  | 1:B:76:SER:HB2   | 1:B:144:THR:HG23 | 4                   | 0.58     | 0.23                | 0.6        |
| (1,251)  | 1:A:89:LEU:HG    | 1:A:90:LYS:H     | 4                   | 0.52     | 0.13                | 0.52       |
| (1,1118) | 1:B:89:LEU:HG    | 1:B:90:LYS:H     | 4                   | 0.52     | 0.13                | 0.52       |
| (1,244)  | 1:A:89:LEU:HD21  | 1:A:88:GLU:H     | 4                   | 0.51     | 0.07                | 0.52       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,244)  | 1:A:89:LEU:HD22  | 1:A:88:GLU:H     | 4                   | 0.51     | 0.07                | 0.52       |
| (1,244)  | 1:A:89:LEU:HD23  | 1:A:88:GLU:H     | 4                   | 0.51     | 0.07                | 0.52       |
| (1,1111) | 1:B:89:LEU:HD21  | 1:B:88:GLU:H     | 4                   | 0.51     | 0.07                | 0.52       |
| (1,1111) | 1:B:89:LEU:HD22  | 1:B:88:GLU:H     | 4                   | 0.51     | 0.07                | 0.52       |
| (1,1111) | 1:B:89:LEU:HD23  | 1:B:88:GLU:H     | 4                   | 0.51     | 0.07                | 0.52       |
| (1,512)  | 1:A:114:ILE:HD11 | 1:A:113:PHE:HA   | 4                   | 0.5      | 0.12                | 0.48       |
| (1,512)  | 1:A:114:ILE:HD12 | 1:A:113:PHE:HA   | 4                   | 0.5      | 0.12                | 0.48       |
| (1,512)  | 1:A:114:ILE:HD13 | 1:A:113:PHE:HA   | 4                   | 0.5      | 0.12                | 0.48       |
| (1,1379) | 1:B:114:ILE:HD11 | 1:B:113:PHE:HA   | 4                   | 0.5      | 0.12                | 0.48       |
| (1,1379) | 1:B:114:ILE:HD12 | 1:B:113:PHE:HA   | 4                   | 0.5      | 0.12                | 0.48       |
| (1,1379) | 1:B:114:ILE:HD13 | 1:B:113:PHE:HA   | 4                   | 0.5      | 0.12                | 0.48       |
| (1,1756) | 1:A:118:PHE:HA   | 1:B:117:GLU:H    | 4                   | 0.5      | 0.22                | 0.4        |
| (1,192)  | 1:A:84:PHE:HD1   | 1:A:83:HIS:HB3   | 4                   | 0.45     | 0.15                | 0.52       |
| (1,192)  | 1:A:84:PHE:HD2   | 1:A:83:HIS:HB3   | 4                   | 0.45     | 0.15                | 0.52       |
| (1,1059) | 1:B:84:PHE:HD1   | 1:B:83:HIS:HB3   | 4                   | 0.45     | 0.15                | 0.52       |
| (1,1059) | 1:B:84:PHE:HD2   | 1:B:83:HIS:HB3   | 4                   | 0.45     | 0.15                | 0.52       |
| (1,102)  | 1:A:77:VAL:HG11  | 1:A:78:ASN:H     | 4                   | 0.43     | 0.25                | 0.42       |
| (1,102)  | 1:A:77:VAL:HG12  | 1:A:78:ASN:H     | 4                   | 0.43     | 0.25                | 0.42       |
| (1,102)  | 1:A:77:VAL:HG13  | 1:A:78:ASN:H     | 4                   | 0.43     | 0.25                | 0.42       |
| (1,1243) | 1:B:101:HIS:HB2  | 1:B:101:HIS:HD2  | 4                   | 0.43     | 0.08                | 0.47       |
| (1,969)  | 1:B:77:VAL:HG11  | 1:B:78:ASN:H     | 4                   | 0.43     | 0.25                | 0.42       |
| (1,969)  | 1:B:77:VAL:HG12  | 1:B:78:ASN:H     | 4                   | 0.43     | 0.25                | 0.42       |
| (1,969)  | 1:B:77:VAL:HG13  | 1:B:78:ASN:H     | 4                   | 0.43     | 0.25                | 0.42       |
| (1,376)  | 1:A:101:HIS:HB2  | 1:A:101:HIS:HD2  | 4                   | 0.42     | 0.07                | 0.46       |
| (1,473)  | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG21 | 4                   | 0.42     | 0.19                | 0.37       |
| (1,473)  | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG22 | 4                   | 0.42     | 0.19                | 0.37       |
| (1,473)  | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG23 | 4                   | 0.42     | 0.19                | 0.37       |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG21 | 4                   | 0.42     | 0.19                | 0.37       |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG22 | 4                   | 0.42     | 0.19                | 0.37       |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG23 | 4                   | 0.42     | 0.19                | 0.37       |
| (1,193)  | 1:A:84:PHE:HD1   | 1:A:83:HIS:HA    | 4                   | 0.42     | 0.15                | 0.48       |
| (1,193)  | 1:A:84:PHE:HD2   | 1:A:83:HIS:HA    | 4                   | 0.42     | 0.15                | 0.48       |
| (1,1060) | 1:B:84:PHE:HD1   | 1:B:83:HIS:HA    | 4                   | 0.42     | 0.15                | 0.48       |
| (1,1060) | 1:B:84:PHE:HD2   | 1:B:83:HIS:HA    | 4                   | 0.42     | 0.15                | 0.48       |
| (1,1440) | 1:B:119:HIS:HA   | 1:B:119:HIS:HD2  | 4                   | 0.35     | 0.08                | 0.38       |
| (1,573)  | 1:A:119:HIS:HA   | 1:A:119:HIS:HD2  | 4                   | 0.32     | 0.09                | 0.34       |
| (1,494)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HD1  | 4                   | 0.31     | 0.05                | 0.3        |
| (1,494)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HD2  | 4                   | 0.31     | 0.05                | 0.3        |
| (1,1361) | 1:B:113:PHE:HA   | 1:B:113:PHE:HD1  | 4                   | 0.31     | 0.06                | 0.3        |
| (1,1361) | 1:B:113:PHE:HA   | 1:B:113:PHE:HD2  | 4                   | 0.31     | 0.06                | 0.3        |
| (1,1476) | 1:B:123:ARG:HA   | 1:B:123:ARG:HD2  | 4                   | 0.3      | 0.06                | 0.3        |
| (1,1476) | 1:B:123:ARG:HA   | 1:B:123:ARG:HD3  | 4                   | 0.3      | 0.06                | 0.3        |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,609)  | 1:A:123:ARG:HA   | 1:A:123:ARG:HD2 | 4                   | 0.3      | 0.06                | 0.3        |
| (1,609)  | 1:A:123:ARG:HA   | 1:A:123:ARG:HD3 | 4                   | 0.3      | 0.06                | 0.3        |
| (1,311)  | 1:A:96:ASP:HB2   | 1:A:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,311)  | 1:A:96:ASP:HB3   | 1:A:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,313)  | 1:A:96:ASP:HB2   | 1:A:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,313)  | 1:A:96:ASP:HB3   | 1:A:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,314)  | 1:A:96:ASP:HB2   | 1:A:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,314)  | 1:A:96:ASP:HB3   | 1:A:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,1178) | 1:B:96:ASP:HB2   | 1:B:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,1178) | 1:B:96:ASP:HB3   | 1:B:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,1180) | 1:B:96:ASP:HB2   | 1:B:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,1180) | 1:B:96:ASP:HB3   | 1:B:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,1181) | 1:B:96:ASP:HB2   | 1:B:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,1181) | 1:B:96:ASP:HB3   | 1:B:96:ASP:H    | 4                   | 0.29     | 0.02                | 0.3        |
| (1,487)  | 1:A:113:PHE:H    | 1:A:112:GLY:H   | 4                   | 0.28     | 0.02                | 0.28       |
| (1,1354) | 1:B:113:PHE:H    | 1:B:112:GLY:H   | 4                   | 0.28     | 0.02                | 0.28       |
| (1,510)  | 1:A:114:ILE:HG21 | 1:A:111:HIS:H   | 4                   | 0.26     | 0.16                | 0.22       |
| (1,510)  | 1:A:114:ILE:HG22 | 1:A:111:HIS:H   | 4                   | 0.26     | 0.16                | 0.22       |
| (1,510)  | 1:A:114:ILE:HG23 | 1:A:111:HIS:H   | 4                   | 0.26     | 0.16                | 0.22       |
| (1,1377) | 1:B:114:ILE:HG21 | 1:B:111:HIS:H   | 4                   | 0.26     | 0.16                | 0.22       |
| (1,1377) | 1:B:114:ILE:HG22 | 1:B:111:HIS:H   | 4                   | 0.26     | 0.16                | 0.22       |
| (1,1377) | 1:B:114:ILE:HG23 | 1:B:111:HIS:H   | 4                   | 0.26     | 0.16                | 0.22       |
| (1,1527) | 1:B:126:ALA:HA   | 1:B:128:VAL:H   | 4                   | 0.26     | 0.22                | 0.16       |
| (1,572)  | 1:A:119:HIS:HB2  | 1:A:119:HIS:HA  | 4                   | 0.26     | 0.05                | 0.29       |
| (1,1439) | 1:B:119:HIS:HB2  | 1:B:119:HIS:HA  | 4                   | 0.26     | 0.04                | 0.28       |
| (1,1146) | 1:B:92:LYS:H     | 1:B:99:GLU:H    | 4                   | 0.25     | 0.1                 | 0.26       |
| (1,279)  | 1:A:92:LYS:H     | 1:A:99:GLU:H    | 4                   | 0.25     | 0.1                 | 0.25       |
| (1,120)  | 1:A:78:ASN:HA    | 1:A:78:ASN:HB3  | 4                   | 0.24     | 0.01                | 0.24       |
| (1,987)  | 1:B:78:ASN:HA    | 1:B:78:ASN:HB3  | 4                   | 0.24     | 0.01                | 0.24       |
| (1,1280) | 1:B:105:GLU:HG2  | 1:B:105:GLU:H   | 4                   | 0.22     | 0.06                | 0.24       |
| (1,1280) | 1:B:105:GLU:HG3  | 1:B:105:GLU:H   | 4                   | 0.22     | 0.06                | 0.24       |
| (1,390)  | 1:A:102:GLY:HA2  | 1:A:103:LYS:H   | 4                   | 0.21     | 0.06                | 0.22       |
| (1,1257) | 1:B:102:GLY:HA2  | 1:B:103:LYS:H   | 4                   | 0.21     | 0.06                | 0.22       |
| (1,241)  | 1:A:89:LEU:H     | 1:A:88:GLU:H    | 4                   | 0.2      | 0.08                | 0.2        |
| (1,242)  | 1:A:89:LEU:H     | 1:A:88:GLU:H    | 4                   | 0.2      | 0.08                | 0.2        |
| (1,129)  | 1:A:78:ASN:HB3   | 1:A:79:LEU:H    | 4                   | 0.18     | 0.05                | 0.18       |
| (1,996)  | 1:B:78:ASN:HB3   | 1:B:79:LEU:H    | 4                   | 0.18     | 0.05                | 0.18       |
| (1,250)  | 1:A:89:LEU:HD21  | 1:A:89:LEU:H    | 4                   | 0.17     | 0.03                | 0.16       |
| (1,250)  | 1:A:89:LEU:HD22  | 1:A:89:LEU:H    | 4                   | 0.17     | 0.03                | 0.16       |
| (1,250)  | 1:A:89:LEU:HD23  | 1:A:89:LEU:H    | 4                   | 0.17     | 0.03                | 0.16       |
| (1,1117) | 1:B:89:LEU:HD21  | 1:B:89:LEU:H    | 4                   | 0.17     | 0.03                | 0.16       |
| (1,1117) | 1:B:89:LEU:HD22  | 1:B:89:LEU:H    | 4                   | 0.17     | 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1117) | 1:B:89:LEU:HD23 | 1:B:89:LEU:H    | 4                   | 0.17     | 0.03                | 0.16       |
| (1,482)  | 1:A:113:PHE:HD1 | 1:A:107:ARG:HA  | 4                   | 0.17     | 0.06                | 0.16       |
| (1,482)  | 1:A:113:PHE:HD2 | 1:A:107:ARG:HA  | 4                   | 0.17     | 0.06                | 0.16       |
| (1,1349) | 1:B:113:PHE:HD1 | 1:B:107:ARG:HA  | 4                   | 0.17     | 0.06                | 0.16       |
| (1,1349) | 1:B:113:PHE:HD2 | 1:B:107:ARG:HA  | 4                   | 0.17     | 0.06                | 0.16       |
| (1,77)   | 1:A:76:SER:HB2  | 1:A:146:ASP:HB3 | 4                   | 0.14     | 0.04                | 0.12       |
| (1,944)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB3 | 4                   | 0.14     | 0.03                | 0.12       |
| (1,425)  | 1:A:107:ARG:HA  | 1:A:107:ARG:H   | 4                   | 0.13     | 0.03                | 0.12       |
| (1,1292) | 1:B:107:ARG:HA  | 1:B:107:ARG:H   | 4                   | 0.13     | 0.03                | 0.12       |
| (1,1399) | 1:B:115:SER:HB3 | 1:B:116:ARG:H   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,45)   | 1:A:75:PHE:HA   | 1:A:74:ARG:HG2  | 3                   | 1.42     | 0.05                | 1.43       |
| (1,45)   | 1:A:75:PHE:HA   | 1:A:74:ARG:HG3  | 3                   | 1.42     | 0.05                | 1.43       |
| (1,912)  | 1:B:75:PHE:HA   | 1:B:74:ARG:HG2  | 3                   | 1.42     | 0.05                | 1.43       |
| (1,912)  | 1:B:75:PHE:HA   | 1:B:74:ARG:HG3  | 3                   | 1.42     | 0.05                | 1.43       |
| (1,642)  | 1:A:125:PRO:HD3 | 1:A:122:TYR:HD1 | 3                   | 1.39     | 0.51                | 1.5        |
| (1,642)  | 1:A:125:PRO:HD3 | 1:A:122:TYR:HD2 | 3                   | 1.39     | 0.51                | 1.5        |
| (1,1509) | 1:B:125:PRO:HD3 | 1:B:122:TYR:HD1 | 3                   | 1.39     | 0.51                | 1.5        |
| (1,1509) | 1:B:125:PRO:HD3 | 1:B:122:TYR:HD2 | 3                   | 1.39     | 0.51                | 1.5        |
| (1,946)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE1  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,946)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE2  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,946)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE3  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,946)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE1  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,946)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE2  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,946)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE3  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,946)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE1  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,946)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE2  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,946)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE3  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,951)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE1  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,951)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE2  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,951)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE3  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,951)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE1  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,951)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE2  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,951)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE3  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,951)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE1  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,951)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE2  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,951)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE3  | 3                   | 1.19     | 0.29                | 1.36       |
| (1,79)   | 1:A:77:VAL:HG21 | 1:A:68:MET:HE1  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,79)   | 1:A:77:VAL:HG21 | 1:A:68:MET:HE2  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,79)   | 1:A:77:VAL:HG21 | 1:A:68:MET:HE3  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,79)   | 1:A:77:VAL:HG22 | 1:A:68:MET:HE1  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,79)   | 1:A:77:VAL:HG22 | 1:A:68:MET:HE2  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,79)   | 1:A:77:VAL:HG22 | 1:A:68:MET:HE3  | 3                   | 1.18     | 0.29                | 1.35       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,79)   | 1:A:77:VAL:HG23 | 1:A:68:MET:HE1  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,79)   | 1:A:77:VAL:HG23 | 1:A:68:MET:HE2  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,79)   | 1:A:77:VAL:HG23 | 1:A:68:MET:HE3  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,84)   | 1:A:77:VAL:HG21 | 1:A:68:MET:HE1  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,84)   | 1:A:77:VAL:HG21 | 1:A:68:MET:HE2  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,84)   | 1:A:77:VAL:HG21 | 1:A:68:MET:HE3  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,84)   | 1:A:77:VAL:HG22 | 1:A:68:MET:HE1  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,84)   | 1:A:77:VAL:HG22 | 1:A:68:MET:HE2  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,84)   | 1:A:77:VAL:HG22 | 1:A:68:MET:HE3  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,84)   | 1:A:77:VAL:HG23 | 1:A:68:MET:HE1  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,84)   | 1:A:77:VAL:HG23 | 1:A:68:MET:HE2  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,84)   | 1:A:77:VAL:HG23 | 1:A:68:MET:HE3  | 3                   | 1.18     | 0.29                | 1.35       |
| (1,739)  | 1:A:135:SER:HB3 | 1:A:145:VAL:HA  | 3                   | 0.96     | 0.03                | 0.96       |
| (1,1606) | 1:B:135:SER:HB3 | 1:B:145:VAL:HA  | 3                   | 0.96     | 0.03                | 0.96       |
| (1,18)   | 1:A:70:LEU:HD11 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,18)   | 1:A:70:LEU:HD12 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,18)   | 1:A:70:LEU:HD13 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,18)   | 1:A:70:LEU:HD21 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,18)   | 1:A:70:LEU:HD22 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,18)   | 1:A:70:LEU:HD23 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,19)   | 1:A:70:LEU:HD11 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,19)   | 1:A:70:LEU:HD12 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,19)   | 1:A:70:LEU:HD13 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,19)   | 1:A:70:LEU:HD21 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,19)   | 1:A:70:LEU:HD22 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,19)   | 1:A:70:LEU:HD23 | 1:A:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,885)  | 1:B:70:LEU:HD11 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,885)  | 1:B:70:LEU:HD12 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,885)  | 1:B:70:LEU:HD13 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,885)  | 1:B:70:LEU:HD21 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,885)  | 1:B:70:LEU:HD22 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,885)  | 1:B:70:LEU:HD23 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,886)  | 1:B:70:LEU:HD11 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,886)  | 1:B:70:LEU:HD12 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,886)  | 1:B:70:LEU:HD13 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,886)  | 1:B:70:LEU:HD21 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,886)  | 1:B:70:LEU:HD22 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,886)  | 1:B:70:LEU:HD23 | 1:B:70:LEU:H    | 3                   | 0.94     | 0.51                | 0.62       |
| (1,859)  | 1:A:150:LYS:H   | 1:A:150:LYS:HG2 | 3                   | 0.9      | 0.03                | 0.89       |
| (1,859)  | 1:A:150:LYS:H   | 1:A:150:LYS:HG3 | 3                   | 0.9      | 0.03                | 0.89       |
| (1,1726) | 1:B:150:LYS:H   | 1:B:150:LYS:HG2 | 3                   | 0.89     | 0.04                | 0.89       |
| (1,1726) | 1:B:150:LYS:H   | 1:B:150:LYS:HG3 | 3                   | 0.89     | 0.04                | 0.89       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,709)  | 1:A:132:THR:HB  | 1:A:147:GLY:HA3  | 3                   | 0.87     | 0.06                | 0.86       |
| (1,1576) | 1:B:132:THR:HB  | 1:B:147:GLY:HA3  | 3                   | 0.87     | 0.06                | 0.86       |
| (1,552)  | 1:A:118:PHE:HE1 | 1:A:103:LYS:H    | 3                   | 0.8      | 0.79                | 0.39       |
| (1,552)  | 1:A:118:PHE:HE2 | 1:A:103:LYS:H    | 3                   | 0.8      | 0.79                | 0.39       |
| (1,1419) | 1:B:118:PHE:HE1 | 1:B:103:LYS:H    | 3                   | 0.8      | 0.79                | 0.39       |
| (1,1419) | 1:B:118:PHE:HE2 | 1:B:103:LYS:H    | 3                   | 0.8      | 0.79                | 0.39       |
| (1,526)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD11 | 3                   | 0.76     | 0.46                | 1.05       |
| (1,526)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD12 | 3                   | 0.76     | 0.46                | 1.05       |
| (1,526)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD13 | 3                   | 0.76     | 0.46                | 1.05       |
| (1,977)  | 1:B:77:VAL:HG11 | 1:B:98:ILE:HD11  | 3                   | 0.75     | 0.16                | 0.73       |
| (1,977)  | 1:B:77:VAL:HG11 | 1:B:98:ILE:HD12  | 3                   | 0.75     | 0.16                | 0.73       |
| (1,977)  | 1:B:77:VAL:HG11 | 1:B:98:ILE:HD13  | 3                   | 0.75     | 0.16                | 0.73       |
| (1,977)  | 1:B:77:VAL:HG12 | 1:B:98:ILE:HD11  | 3                   | 0.75     | 0.16                | 0.73       |
| (1,977)  | 1:B:77:VAL:HG12 | 1:B:98:ILE:HD12  | 3                   | 0.75     | 0.16                | 0.73       |
| (1,977)  | 1:B:77:VAL:HG12 | 1:B:98:ILE:HD13  | 3                   | 0.75     | 0.16                | 0.73       |
| (1,977)  | 1:B:77:VAL:HG13 | 1:B:98:ILE:HD11  | 3                   | 0.75     | 0.16                | 0.73       |
| (1,977)  | 1:B:77:VAL:HG13 | 1:B:98:ILE:HD12  | 3                   | 0.75     | 0.16                | 0.73       |
| (1,977)  | 1:B:77:VAL:HG13 | 1:B:98:ILE:HD13  | 3                   | 0.75     | 0.16                | 0.73       |
| (1,110)  | 1:A:77:VAL:HG11 | 1:A:98:ILE:HD11  | 3                   | 0.74     | 0.15                | 0.73       |
| (1,110)  | 1:A:77:VAL:HG11 | 1:A:98:ILE:HD12  | 3                   | 0.74     | 0.15                | 0.73       |
| (1,110)  | 1:A:77:VAL:HG11 | 1:A:98:ILE:HD13  | 3                   | 0.74     | 0.15                | 0.73       |
| (1,110)  | 1:A:77:VAL:HG12 | 1:A:98:ILE:HD11  | 3                   | 0.74     | 0.15                | 0.73       |
| (1,110)  | 1:A:77:VAL:HG12 | 1:A:98:ILE:HD12  | 3                   | 0.74     | 0.15                | 0.73       |
| (1,110)  | 1:A:77:VAL:HG12 | 1:A:98:ILE:HD13  | 3                   | 0.74     | 0.15                | 0.73       |
| (1,110)  | 1:A:77:VAL:HG13 | 1:A:98:ILE:HD11  | 3                   | 0.74     | 0.15                | 0.73       |
| (1,110)  | 1:A:77:VAL:HG13 | 1:A:98:ILE:HD12  | 3                   | 0.74     | 0.15                | 0.73       |
| (1,110)  | 1:A:77:VAL:HG13 | 1:A:98:ILE:HD13  | 3                   | 0.74     | 0.15                | 0.73       |
| (1,50)   | 1:A:75:PHE:HD1  | 1:A:75:PHE:H     | 3                   | 0.7      | 0.11                | 0.74       |
| (1,50)   | 1:A:75:PHE:HD2  | 1:A:75:PHE:H     | 3                   | 0.7      | 0.11                | 0.74       |
| (1,917)  | 1:B:75:PHE:HD1  | 1:B:75:PHE:H     | 3                   | 0.7      | 0.11                | 0.74       |
| (1,917)  | 1:B:75:PHE:HD2  | 1:B:75:PHE:H     | 3                   | 0.7      | 0.11                | 0.74       |
| (1,17)   | 1:A:70:LEU:H    | 1:A:70:LEU:HB3   | 3                   | 0.68     | 0.07                | 0.66       |
| (1,884)  | 1:B:70:LEU:H    | 1:B:70:LEU:HB3   | 3                   | 0.68     | 0.07                | 0.66       |
| (1,296)  | 1:A:94:LEU:H    | 1:A:99:GLU:H     | 3                   | 0.68     | 0.36                | 0.75       |
| (1,1163) | 1:B:94:LEU:H    | 1:B:99:GLU:H     | 3                   | 0.68     | 0.36                | 0.75       |
| (1,35)   | 1:A:73:ASP:H    | 1:A:74:ARG:HB3   | 3                   | 0.65     | 0.08                | 0.62       |
| (1,902)  | 1:B:73:ASP:H    | 1:B:74:ARG:HB3   | 3                   | 0.65     | 0.08                | 0.62       |
| (1,950)  | 1:B:77:VAL:HG11 | 1:B:68:MET:HA    | 3                   | 0.6      | 0.28                | 0.49       |
| (1,950)  | 1:B:77:VAL:HG12 | 1:B:68:MET:HA    | 3                   | 0.6      | 0.28                | 0.49       |
| (1,950)  | 1:B:77:VAL:HG13 | 1:B:68:MET:HA    | 3                   | 0.6      | 0.28                | 0.49       |
| (1,83)   | 1:A:77:VAL:HG11 | 1:A:68:MET:HA    | 3                   | 0.6      | 0.28                | 0.49       |
| (1,83)   | 1:A:77:VAL:HG12 | 1:A:68:MET:HA    | 3                   | 0.6      | 0.28                | 0.49       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,83)   | 1:A:77:VAL:HG13 | 1:A:68:MET:HA   | 3                   | 0.6      | 0.28                | 0.49       |
| (1,565)  | 1:A:118:PHE:HB2 | 1:A:119:HIS:H   | 3                   | 0.59     | 0.08                | 0.57       |
| (1,1432) | 1:B:118:PHE:HB2 | 1:B:119:HIS:H   | 3                   | 0.59     | 0.08                | 0.57       |
| (1,1020) | 1:B:81:VAL:HG11 | 1:B:80:ASP:HA   | 3                   | 0.56     | 0.03                | 0.54       |
| (1,1020) | 1:B:81:VAL:HG12 | 1:B:80:ASP:HA   | 3                   | 0.56     | 0.03                | 0.54       |
| (1,1020) | 1:B:81:VAL:HG13 | 1:B:80:ASP:HA   | 3                   | 0.56     | 0.03                | 0.54       |
| (1,153)  | 1:A:81:VAL:HG11 | 1:A:80:ASP:HA   | 3                   | 0.56     | 0.02                | 0.54       |
| (1,153)  | 1:A:81:VAL:HG12 | 1:A:80:ASP:HA   | 3                   | 0.56     | 0.02                | 0.54       |
| (1,153)  | 1:A:81:VAL:HG13 | 1:A:80:ASP:HA   | 3                   | 0.56     | 0.02                | 0.54       |
| (1,154)  | 1:A:81:VAL:HG21 | 1:A:81:VAL:HA   | 3                   | 0.53     | 0.04                | 0.51       |
| (1,154)  | 1:A:81:VAL:HG22 | 1:A:81:VAL:HA   | 3                   | 0.53     | 0.04                | 0.51       |
| (1,154)  | 1:A:81:VAL:HG23 | 1:A:81:VAL:HA   | 3                   | 0.53     | 0.04                | 0.51       |
| (1,1021) | 1:B:81:VAL:HG21 | 1:B:81:VAL:HA   | 3                   | 0.52     | 0.05                | 0.49       |
| (1,1021) | 1:B:81:VAL:HG22 | 1:B:81:VAL:HA   | 3                   | 0.52     | 0.05                | 0.49       |
| (1,1021) | 1:B:81:VAL:HG23 | 1:B:81:VAL:HA   | 3                   | 0.52     | 0.05                | 0.49       |
| (1,383)  | 1:A:101:HIS:HA  | 1:A:119:HIS:HD2 | 3                   | 0.48     | 0.25                | 0.45       |
| (1,1250) | 1:B:101:HIS:HA  | 1:B:119:HIS:HD2 | 3                   | 0.48     | 0.27                | 0.4        |
| (1,3)    | 1:A:66:SER:HB2  | 1:A:66:SER:H    | 3                   | 0.44     | 0.16                | 0.45       |
| (1,870)  | 1:B:66:SER:HB2  | 1:B:66:SER:H    | 3                   | 0.44     | 0.16                | 0.45       |
| (1,418)  | 1:A:105:GLU:HG2 | 1:A:115:SER:HB3 | 3                   | 0.43     | 0.3                 | 0.28       |
| (1,418)  | 1:A:105:GLU:HG3 | 1:A:115:SER:HB3 | 3                   | 0.43     | 0.3                 | 0.28       |
| (1,1285) | 1:B:105:GLU:HG2 | 1:B:115:SER:HB3 | 3                   | 0.43     | 0.3                 | 0.28       |
| (1,1285) | 1:B:105:GLU:HG3 | 1:B:115:SER:HB3 | 3                   | 0.43     | 0.3                 | 0.28       |
| (1,863)  | 1:A:150:LYS:H   | 1:A:151:GLN:H   | 3                   | 0.43     | 0.27                | 0.31       |
| (1,4)    | 1:A:66:SER:HA   | 1:A:79:LEU:HD11 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,4)    | 1:A:66:SER:HA   | 1:A:79:LEU:HD12 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,4)    | 1:A:66:SER:HA   | 1:A:79:LEU:HD13 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,4)    | 1:A:66:SER:HA   | 1:A:79:LEU:HD21 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,4)    | 1:A:66:SER:HA   | 1:A:79:LEU:HD22 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,4)    | 1:A:66:SER:HA   | 1:A:79:LEU:HD23 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,871)  | 1:B:66:SER:HA   | 1:B:79:LEU:HD11 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,871)  | 1:B:66:SER:HA   | 1:B:79:LEU:HD12 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,871)  | 1:B:66:SER:HA   | 1:B:79:LEU:HD13 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,871)  | 1:B:66:SER:HA   | 1:B:79:LEU:HD21 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,871)  | 1:B:66:SER:HA   | 1:B:79:LEU:HD22 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,871)  | 1:B:66:SER:HA   | 1:B:79:LEU:HD23 | 3                   | 0.43     | 0.09                | 0.41       |
| (1,1730) | 1:B:150:LYS:H   | 1:B:151:GLN:H   | 3                   | 0.43     | 0.26                | 0.31       |
| (1,881)  | 1:B:68:MET:HE1  | 1:B:122:TYR:HD1 | 3                   | 0.41     | 0.17                | 0.37       |
| (1,881)  | 1:B:68:MET:HE1  | 1:B:122:TYR:HD2 | 3                   | 0.41     | 0.17                | 0.37       |
| (1,881)  | 1:B:68:MET:HE2  | 1:B:122:TYR:HD1 | 3                   | 0.41     | 0.17                | 0.37       |
| (1,881)  | 1:B:68:MET:HE2  | 1:B:122:TYR:HD2 | 3                   | 0.41     | 0.17                | 0.37       |
| (1,881)  | 1:B:68:MET:HE3  | 1:B:122:TYR:HD1 | 3                   | 0.41     | 0.17                | 0.37       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,881)  | 1:B:68:MET:HE3  | 1:B:122:TYR:HD2  | 3                   | 0.41     | 0.17                | 0.37       |
| (1,14)   | 1:A:68:MET:HE1  | 1:A:122:TYR:HD1  | 3                   | 0.41     | 0.17                | 0.36       |
| (1,14)   | 1:A:68:MET:HE1  | 1:A:122:TYR:HD2  | 3                   | 0.41     | 0.17                | 0.36       |
| (1,14)   | 1:A:68:MET:HE2  | 1:A:122:TYR:HD1  | 3                   | 0.41     | 0.17                | 0.36       |
| (1,14)   | 1:A:68:MET:HE2  | 1:A:122:TYR:HD2  | 3                   | 0.41     | 0.17                | 0.36       |
| (1,14)   | 1:A:68:MET:HE3  | 1:A:122:TYR:HD1  | 3                   | 0.41     | 0.17                | 0.36       |
| (1,14)   | 1:A:68:MET:HE3  | 1:A:122:TYR:HD2  | 3                   | 0.41     | 0.17                | 0.36       |
| (1,1199) | 1:B:97:VAL:HA   | 1:B:124:ILE:HG12 | 3                   | 0.37     | 0.07                | 0.41       |
| (1,1199) | 1:B:97:VAL:HA   | 1:B:124:ILE:HG13 | 3                   | 0.37     | 0.07                | 0.41       |
| (1,332)  | 1:A:97:VAL:HA   | 1:A:124:ILE:HG12 | 3                   | 0.37     | 0.07                | 0.41       |
| (1,332)  | 1:A:97:VAL:HA   | 1:A:124:ILE:HG13 | 3                   | 0.37     | 0.07                | 0.41       |
| (1,9)    | 1:A:68:MET:HE1  | 1:A:68:MET:H     | 3                   | 0.36     | 0.16                | 0.29       |
| (1,9)    | 1:A:68:MET:HE2  | 1:A:68:MET:H     | 3                   | 0.36     | 0.16                | 0.29       |
| (1,9)    | 1:A:68:MET:HE3  | 1:A:68:MET:H     | 3                   | 0.36     | 0.16                | 0.29       |
| (1,876)  | 1:B:68:MET:HE1  | 1:B:68:MET:H     | 3                   | 0.35     | 0.17                | 0.29       |
| (1,876)  | 1:B:68:MET:HE2  | 1:B:68:MET:H     | 3                   | 0.35     | 0.17                | 0.29       |
| (1,876)  | 1:B:68:MET:HE3  | 1:B:68:MET:H     | 3                   | 0.35     | 0.17                | 0.29       |
| (1,660)  | 1:A:126:ALA:HA  | 1:A:128:VAL:H    | 3                   | 0.31     | 0.22                | 0.17       |
| (1,787)  | 1:A:143:LEU:H   | 1:A:79:LEU:H     | 3                   | 0.31     | 0.15                | 0.35       |
| (1,1654) | 1:B:143:LEU:H   | 1:B:79:LEU:H     | 3                   | 0.31     | 0.15                | 0.35       |
| (1,42)   | 1:A:74:ARG:H    | 1:A:74:ARG:HB2   | 3                   | 0.29     | 0.05                | 0.31       |
| (1,909)  | 1:B:74:ARG:H    | 1:B:74:ARG:HB2   | 3                   | 0.29     | 0.05                | 0.31       |
| (1,1331) | 1:B:111:HIS:H   | 1:B:111:HIS:HD2  | 3                   | 0.29     | 0.13                | 0.2        |
| (1,471)  | 1:A:111:HIS:H   | 1:A:112:GLY:H    | 3                   | 0.28     | 0.16                | 0.17       |
| (1,1338) | 1:B:111:HIS:H   | 1:B:112:GLY:H    | 3                   | 0.28     | 0.16                | 0.17       |
| (1,37)   | 1:A:74:ARG:H    | 1:A:73:ASP:H     | 3                   | 0.26     | 0.04                | 0.28       |
| (1,38)   | 1:A:74:ARG:H    | 1:A:73:ASP:H     | 3                   | 0.26     | 0.04                | 0.28       |
| (1,904)  | 1:B:74:ARG:H    | 1:B:73:ASP:H     | 3                   | 0.26     | 0.04                | 0.28       |
| (1,905)  | 1:B:74:ARG:H    | 1:B:73:ASP:H     | 3                   | 0.26     | 0.04                | 0.28       |
| (1,282)  | 1:A:93:VAL:H    | 1:A:92:LYS:HG2   | 3                   | 0.25     | 0.11                | 0.19       |
| (1,282)  | 1:A:93:VAL:H    | 1:A:92:LYS:HG3   | 3                   | 0.25     | 0.11                | 0.19       |
| (1,413)  | 1:A:105:GLU:HG2 | 1:A:105:GLU:H    | 3                   | 0.25     | 0.02                | 0.25       |
| (1,413)  | 1:A:105:GLU:HG3 | 1:A:105:GLU:H    | 3                   | 0.25     | 0.02                | 0.25       |
| (1,1149) | 1:B:93:VAL:H    | 1:B:92:LYS:HG2   | 3                   | 0.25     | 0.11                | 0.19       |
| (1,1149) | 1:B:93:VAL:H    | 1:B:92:LYS:HG3   | 3                   | 0.25     | 0.11                | 0.19       |
| (1,485)  | 1:A:113:PHE:HA  | 1:A:108:GLN:HA   | 3                   | 0.24     | 0.07                | 0.25       |
| (1,1352) | 1:B:113:PHE:HA  | 1:B:108:GLN:HA   | 3                   | 0.24     | 0.07                | 0.25       |
| (1,80)   | 1:A:77:VAL:HA   | 1:A:68:MET:HA    | 3                   | 0.24     | 0.05                | 0.27       |
| (1,947)  | 1:B:77:VAL:HA   | 1:B:68:MET:HA    | 3                   | 0.24     | 0.05                | 0.27       |
| (1,1108) | 1:B:89:LEU:H    | 1:B:88:GLU:H     | 3                   | 0.23     | 0.06                | 0.25       |
| (1,1109) | 1:B:89:LEU:H    | 1:B:88:GLU:H     | 3                   | 0.23     | 0.06                | 0.25       |
| (1,57)   | 1:A:75:PHE:H    | 1:A:149:ARG:H    | 3                   | 0.22     | 0.14                | 0.14       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,924)  | 1:B:75:PHE:H     | 1:B:149:ARG:H   | 3                   | 0.22     | 0.14                | 0.14       |
| (1,48)   | 1:A:75:PHE:HA    | 1:A:75:PHE:HB3  | 3                   | 0.22     | 0.07                | 0.22       |
| (1,275)  | 1:A:92:LYS:H     | 1:A:92:LYS:HG2  | 3                   | 0.22     | 0.05                | 0.24       |
| (1,275)  | 1:A:92:LYS:H     | 1:A:92:LYS:HG3  | 3                   | 0.22     | 0.05                | 0.24       |
| (1,915)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HB3  | 3                   | 0.22     | 0.07                | 0.22       |
| (1,1142) | 1:B:92:LYS:H     | 1:B:92:LYS:HG2  | 3                   | 0.22     | 0.05                | 0.24       |
| (1,1142) | 1:B:92:LYS:H     | 1:B:92:LYS:HG3  | 3                   | 0.22     | 0.05                | 0.24       |
| (1,860)  | 1:A:150:LYS:H    | 1:A:151:GLN:H   | 3                   | 0.21     | 0.07                | 0.18       |
| (1,1672) | 1:B:144:THR:HG21 | 1:B:145:VAL:H   | 3                   | 0.21     | 0.07                | 0.22       |
| (1,1672) | 1:B:144:THR:HG22 | 1:B:145:VAL:H   | 3                   | 0.21     | 0.07                | 0.22       |
| (1,1672) | 1:B:144:THR:HG23 | 1:B:145:VAL:H   | 3                   | 0.21     | 0.07                | 0.22       |
| (1,1727) | 1:B:150:LYS:H    | 1:B:151:GLN:H   | 3                   | 0.21     | 0.08                | 0.18       |
| (1,805)  | 1:A:144:THR:HG21 | 1:A:145:VAL:H   | 3                   | 0.2      | 0.07                | 0.21       |
| (1,805)  | 1:A:144:THR:HG22 | 1:A:145:VAL:H   | 3                   | 0.2      | 0.07                | 0.21       |
| (1,805)  | 1:A:144:THR:HG23 | 1:A:145:VAL:H   | 3                   | 0.2      | 0.07                | 0.21       |
| (1,85)   | 1:A:77:VAL:HB    | 1:A:75:PHE:HD1  | 3                   | 0.19     | 0.01                | 0.19       |
| (1,85)   | 1:A:77:VAL:HB    | 1:A:75:PHE:HD2  | 3                   | 0.19     | 0.01                | 0.19       |
| (1,952)  | 1:B:77:VAL:HB    | 1:B:75:PHE:HD1  | 3                   | 0.19     | 0.01                | 0.19       |
| (1,952)  | 1:B:77:VAL:HB    | 1:B:75:PHE:HD2  | 3                   | 0.19     | 0.01                | 0.19       |
| (1,614)  | 1:A:124:ILE:HD11 | 1:A:96:ASP:H    | 3                   | 0.18     | 0.05                | 0.15       |
| (1,614)  | 1:A:124:ILE:HD12 | 1:A:96:ASP:H    | 3                   | 0.18     | 0.05                | 0.15       |
| (1,614)  | 1:A:124:ILE:HD13 | 1:A:96:ASP:H    | 3                   | 0.18     | 0.05                | 0.15       |
| (1,731)  | 1:A:134:THR:HG21 | 1:A:135:SER:H   | 3                   | 0.18     | 0.03                | 0.19       |
| (1,731)  | 1:A:134:THR:HG22 | 1:A:135:SER:H   | 3                   | 0.18     | 0.03                | 0.19       |
| (1,731)  | 1:A:134:THR:HG23 | 1:A:135:SER:H   | 3                   | 0.18     | 0.03                | 0.19       |
| (1,1481) | 1:B:124:ILE:HD11 | 1:B:96:ASP:H    | 3                   | 0.18     | 0.04                | 0.15       |
| (1,1481) | 1:B:124:ILE:HD12 | 1:B:96:ASP:H    | 3                   | 0.18     | 0.04                | 0.15       |
| (1,1481) | 1:B:124:ILE:HD13 | 1:B:96:ASP:H    | 3                   | 0.18     | 0.04                | 0.15       |
| (1,1598) | 1:B:134:THR:HG21 | 1:B:135:SER:H   | 3                   | 0.18     | 0.03                | 0.19       |
| (1,1598) | 1:B:134:THR:HG22 | 1:B:135:SER:H   | 3                   | 0.18     | 0.03                | 0.19       |
| (1,1598) | 1:B:134:THR:HG23 | 1:B:135:SER:H   | 3                   | 0.18     | 0.03                | 0.19       |
| (1,1622) | 1:B:138:SER:H    | 1:B:137:LEU:H   | 3                   | 0.18     | 0.02                | 0.17       |
| (1,755)  | 1:A:138:SER:H    | 1:A:137:LEU:H   | 3                   | 0.17     | 0.02                | 0.16       |
| (1,942)  | 1:B:76:SER:HB3   | 1:B:146:ASP:HB3 | 3                   | 0.17     | 0.05                | 0.15       |
| (1,75)   | 1:A:76:SER:HB3   | 1:A:146:ASP:HB3 | 3                   | 0.17     | 0.05                | 0.15       |
| (1,656)  | 1:A:125:PRO:HA   | 1:A:127:ASP:H   | 3                   | 0.17     | 0.04                | 0.17       |
| (1,1523) | 1:B:125:PRO:HA   | 1:B:127:ASP:H   | 3                   | 0.17     | 0.04                | 0.17       |
| (1,794)  | 1:A:144:THR:HG21 | 1:A:78:ASN:HA   | 3                   | 0.16     | 0.04                | 0.18       |
| (1,794)  | 1:A:144:THR:HG22 | 1:A:78:ASN:HA   | 3                   | 0.16     | 0.04                | 0.18       |
| (1,794)  | 1:A:144:THR:HG23 | 1:A:78:ASN:HA   | 3                   | 0.16     | 0.04                | 0.18       |
| (1,417)  | 1:A:105:GLU:HG2  | 1:A:106:GLU:H   | 3                   | 0.16     | 0.02                | 0.16       |
| (1,417)  | 1:A:105:GLU:HG3  | 1:A:106:GLU:H   | 3                   | 0.16     | 0.02                | 0.16       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1284) | 1:B:105:GLU:HG2 | 1:B:106:GLU:H    | 3                   | 0.16     | 0.02                | 0.16       |
| (1,1284) | 1:B:105:GLU:HG3 | 1:B:106:GLU:H    | 3                   | 0.16     | 0.02                | 0.16       |
| (1,372)  | 1:A:101:HIS:HA  | 1:A:101:HIS:HD2  | 3                   | 0.16     | 0.05                | 0.12       |
| (1,1239) | 1:B:101:HIS:HA  | 1:B:101:HIS:HD2  | 3                   | 0.16     | 0.05                | 0.12       |
| (1,47)   | 1:A:75:PHE:HA   | 1:A:75:PHE:HD1   | 3                   | 0.15     | 0.03                | 0.15       |
| (1,47)   | 1:A:75:PHE:HA   | 1:A:75:PHE:HD2   | 3                   | 0.15     | 0.03                | 0.15       |
| (1,914)  | 1:B:75:PHE:HA   | 1:B:75:PHE:HD1   | 3                   | 0.15     | 0.03                | 0.15       |
| (1,914)  | 1:B:75:PHE:HA   | 1:B:75:PHE:HD2   | 3                   | 0.15     | 0.03                | 0.15       |
| (1,424)  | 1:A:107:ARG:HG2 | 1:A:107:ARG:HA   | 3                   | 0.14     | 0.01                | 0.14       |
| (1,424)  | 1:A:107:ARG:HG3 | 1:A:107:ARG:HA   | 3                   | 0.14     | 0.01                | 0.14       |
| (1,1291) | 1:B:107:ARG:HG2 | 1:B:107:ARG:HA   | 3                   | 0.14     | 0.01                | 0.14       |
| (1,1291) | 1:B:107:ARG:HG3 | 1:B:107:ARG:HA   | 3                   | 0.14     | 0.01                | 0.14       |
| (1,596)  | 1:A:122:TYR:HA  | 1:A:122:TYR:H    | 3                   | 0.14     | 0.01                | 0.14       |
| (1,1463) | 1:B:122:TYR:HA  | 1:B:122:TYR:H    | 3                   | 0.14     | 0.01                | 0.14       |
| (1,374)  | 1:A:101:HIS:HB2 | 1:A:101:HIS:HA   | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,375)  | 1:A:101:HIS:HB2 | 1:A:101:HIS:HA   | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,1241) | 1:B:101:HIS:HB2 | 1:B:101:HIS:HA   | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,1242) | 1:B:101:HIS:HB2 | 1:B:101:HIS:HA   | 3                   | 0.13     | 0.0                 | 0.13       |
| (1,123)  | 1:A:78:ASN:HB3  | 1:A:78:ASN:H     | 3                   | 0.13     | 0.01                | 0.12       |
| (1,990)  | 1:B:78:ASN:HB3  | 1:B:78:ASN:H     | 3                   | 0.13     | 0.01                | 0.12       |
| (1,532)  | 1:A:115:SER:HB3 | 1:A:116:ARG:H    | 3                   | 0.12     | 0.01                | 0.12       |
| (1,1054) | 1:B:83:HIS:HB3  | 1:B:104:HIS:HD2  | 2                   | 1.48     | 0.03                | 1.48       |
| (1,187)  | 1:A:83:HIS:HB3  | 1:A:104:HIS:HD2  | 2                   | 1.48     | 0.04                | 1.48       |
| (1,523)  | 1:A:115:SER:HB3 | 1:A:106:GLU:H    | 2                   | 1.4      | 0.92                | 1.4        |
| (1,1390) | 1:B:115:SER:HB3 | 1:B:106:GLU:H    | 2                   | 1.4      | 0.92                | 1.4        |
| (1,98)   | 1:A:77:VAL:HG11 | 1:A:77:VAL:H     | 2                   | 1.3      | 0.08                | 1.3        |
| (1,98)   | 1:A:77:VAL:HG12 | 1:A:77:VAL:H     | 2                   | 1.3      | 0.08                | 1.3        |
| (1,98)   | 1:A:77:VAL:HG13 | 1:A:77:VAL:H     | 2                   | 1.3      | 0.08                | 1.3        |
| (1,965)  | 1:B:77:VAL:HG11 | 1:B:77:VAL:H     | 2                   | 1.3      | 0.08                | 1.3        |
| (1,965)  | 1:B:77:VAL:HG12 | 1:B:77:VAL:H     | 2                   | 1.3      | 0.08                | 1.3        |
| (1,965)  | 1:B:77:VAL:HG13 | 1:B:77:VAL:H     | 2                   | 1.3      | 0.08                | 1.3        |
| (1,1393) | 1:B:115:SER:HA  | 1:B:114:ILE:HD11 | 2                   | 1.08     | 0.03                | 1.08       |
| (1,1393) | 1:B:115:SER:HA  | 1:B:114:ILE:HD12 | 2                   | 1.08     | 0.03                | 1.08       |
| (1,1393) | 1:B:115:SER:HA  | 1:B:114:ILE:HD13 | 2                   | 1.08     | 0.03                | 1.08       |
| (1,527)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD11 | 2                   | 0.96     | 0.1                 | 0.96       |
| (1,527)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD12 | 2                   | 0.96     | 0.1                 | 0.96       |
| (1,527)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD13 | 2                   | 0.96     | 0.1                 | 0.96       |
| (1,1394) | 1:B:115:SER:HA  | 1:B:114:ILE:HD11 | 2                   | 0.96     | 0.1                 | 0.96       |
| (1,1394) | 1:B:115:SER:HA  | 1:B:114:ILE:HD12 | 2                   | 0.96     | 0.1                 | 0.96       |
| (1,1394) | 1:B:115:SER:HA  | 1:B:114:ILE:HD13 | 2                   | 0.96     | 0.1                 | 0.96       |
| (1,139)  | 1:A:79:LEU:HD11 | 1:A:79:LEU:H     | 2                   | 0.96     | 0.02                | 0.96       |
| (1,139)  | 1:A:79:LEU:HD12 | 1:A:79:LEU:H     | 2                   | 0.96     | 0.02                | 0.96       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,139)  | 1:A:79:LEU:HD13  | 1:A:79:LEU:H    | 2                   | 0.96     | 0.02                | 0.96       |
| (1,139)  | 1:A:79:LEU:HD21  | 1:A:79:LEU:H    | 2                   | 0.96     | 0.02                | 0.96       |
| (1,139)  | 1:A:79:LEU:HD22  | 1:A:79:LEU:H    | 2                   | 0.96     | 0.02                | 0.96       |
| (1,139)  | 1:A:79:LEU:HD23  | 1:A:79:LEU:H    | 2                   | 0.96     | 0.02                | 0.96       |
| (1,140)  | 1:A:79:LEU:HD11  | 1:A:79:LEU:H    | 2                   | 0.96     | 0.02                | 0.96       |
| (1,140)  | 1:A:79:LEU:HD12  | 1:A:79:LEU:H    | 2                   | 0.96     | 0.02                | 0.96       |
| (1,140)  | 1:A:79:LEU:HD13  | 1:A:79:LEU:H    | 2                   | 0.96     | 0.02                | 0.96       |
| (1,140)  | 1:A:79:LEU:HD21  | 1:A:79:LEU:H    | 2                   | 0.96     | 0.02                | 0.96       |
| (1,140)  | 1:A:79:LEU:HD22  | 1:A:79:LEU:H    | 2                   | 0.96     | 0.02                | 0.96       |
| (1,140)  | 1:A:79:LEU:HD23  | 1:A:79:LEU:H    | 2                   | 0.96     | 0.02                | 0.96       |
| (1,1006) | 1:B:79:LEU:HD11  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,1006) | 1:B:79:LEU:HD12  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,1006) | 1:B:79:LEU:HD13  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,1006) | 1:B:79:LEU:HD21  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,1006) | 1:B:79:LEU:HD22  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,1006) | 1:B:79:LEU:HD23  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,1007) | 1:B:79:LEU:HD11  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,1007) | 1:B:79:LEU:HD12  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,1007) | 1:B:79:LEU:HD13  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,1007) | 1:B:79:LEU:HD21  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,1007) | 1:B:79:LEU:HD22  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,1007) | 1:B:79:LEU:HD23  | 1:B:79:LEU:H    | 2                   | 0.95     | 0.02                | 0.95       |
| (1,504)  | 1:A:114:ILE:HD11 | 1:A:107:ARG:HD2 | 2                   | 0.87     | 0.04                | 0.87       |
| (1,504)  | 1:A:114:ILE:HD12 | 1:A:107:ARG:HD2 | 2                   | 0.87     | 0.04                | 0.87       |
| (1,504)  | 1:A:114:ILE:HD13 | 1:A:107:ARG:HD2 | 2                   | 0.87     | 0.04                | 0.87       |
| (1,509)  | 1:A:114:ILE:HG21 | 1:A:109:ASP:H   | 2                   | 0.86     | 0.4                 | 0.86       |
| (1,509)  | 1:A:114:ILE:HG22 | 1:A:109:ASP:H   | 2                   | 0.86     | 0.4                 | 0.86       |
| (1,509)  | 1:A:114:ILE:HG23 | 1:A:109:ASP:H   | 2                   | 0.86     | 0.4                 | 0.86       |
| (1,1371) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HD2 | 2                   | 0.86     | 0.05                | 0.86       |
| (1,1371) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HD2 | 2                   | 0.86     | 0.05                | 0.86       |
| (1,1371) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HD2 | 2                   | 0.86     | 0.05                | 0.86       |
| (1,1376) | 1:B:114:ILE:HG21 | 1:B:109:ASP:H   | 2                   | 0.86     | 0.4                 | 0.86       |
| (1,1376) | 1:B:114:ILE:HG22 | 1:B:109:ASP:H   | 2                   | 0.86     | 0.4                 | 0.86       |
| (1,1376) | 1:B:114:ILE:HG23 | 1:B:109:ASP:H   | 2                   | 0.86     | 0.4                 | 0.86       |
| (1,727)  | 1:A:133:ILE:HG21 | 1:A:145:VAL:HB  | 2                   | 0.84     | 0.52                | 0.84       |
| (1,727)  | 1:A:133:ILE:HG22 | 1:A:145:VAL:HB  | 2                   | 0.84     | 0.52                | 0.84       |
| (1,727)  | 1:A:133:ILE:HG23 | 1:A:145:VAL:HB  | 2                   | 0.84     | 0.52                | 0.84       |
| (1,1594) | 1:B:133:ILE:HG21 | 1:B:145:VAL:HB  | 2                   | 0.83     | 0.52                | 0.83       |
| (1,1594) | 1:B:133:ILE:HG22 | 1:B:145:VAL:HB  | 2                   | 0.83     | 0.52                | 0.83       |
| (1,1594) | 1:B:133:ILE:HG23 | 1:B:145:VAL:HB  | 2                   | 0.83     | 0.52                | 0.83       |
| (1,186)  | 1:A:83:HIS:HB2   | 1:A:104:HIS:HB2 | 2                   | 0.8      | 0.65                | 0.8        |
| (1,269)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG11 | 2                   | 0.8      | 0.02                | 0.8        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,269)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG12  | 2                   | 0.8      | 0.02                | 0.8        |
| (1,269)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG13  | 2                   | 0.8      | 0.02                | 0.8        |
| (1,1136) | 1:B:91:VAL:H     | 1:B:91:VAL:HG11  | 2                   | 0.8      | 0.02                | 0.8        |
| (1,1136) | 1:B:91:VAL:H     | 1:B:91:VAL:HG12  | 2                   | 0.8      | 0.02                | 0.8        |
| (1,1136) | 1:B:91:VAL:H     | 1:B:91:VAL:HG13  | 2                   | 0.8      | 0.02                | 0.8        |
| (1,1053) | 1:B:83:HIS:HB2   | 1:B:104:HIS:HB2  | 2                   | 0.8      | 0.66                | 0.8        |
| (1,449)  | 1:A:109:ASP:HA   | 1:A:111:HIS:H    | 2                   | 0.75     | 0.02                | 0.75       |
| (1,723)  | 1:A:133:ILE:HG21 | 1:A:133:ILE:H    | 2                   | 0.75     | 0.02                | 0.75       |
| (1,723)  | 1:A:133:ILE:HG22 | 1:A:133:ILE:H    | 2                   | 0.75     | 0.02                | 0.75       |
| (1,723)  | 1:A:133:ILE:HG23 | 1:A:133:ILE:H    | 2                   | 0.75     | 0.02                | 0.75       |
| (1,1316) | 1:B:109:ASP:HA   | 1:B:111:HIS:H    | 2                   | 0.75     | 0.02                | 0.75       |
| (1,1590) | 1:B:133:ILE:HG21 | 1:B:133:ILE:H    | 2                   | 0.74     | 0.02                | 0.74       |
| (1,1590) | 1:B:133:ILE:HG22 | 1:B:133:ILE:H    | 2                   | 0.74     | 0.02                | 0.74       |
| (1,1590) | 1:B:133:ILE:HG23 | 1:B:133:ILE:H    | 2                   | 0.74     | 0.02                | 0.74       |
| (1,686)  | 1:A:129:ASP:H    | 1:A:132:THR:HG1  | 2                   | 0.71     | 0.22                | 0.71       |
| (1,571)  | 1:A:119:HIS:HA   | 1:A:101:HIS:HD2  | 2                   | 0.69     | 0.23                | 0.69       |
| (1,699)  | 1:A:132:THR:HG1  | 1:A:132:THR:H    | 2                   | 0.69     | 0.05                | 0.69       |
| (1,1438) | 1:B:119:HIS:HA   | 1:B:101:HIS:HD2  | 2                   | 0.68     | 0.24                | 0.68       |
| (1,1712) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HD11 | 2                   | 0.66     | 0.1                 | 0.66       |
| (1,1712) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HD12 | 2                   | 0.66     | 0.1                 | 0.66       |
| (1,1712) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HD13 | 2                   | 0.66     | 0.1                 | 0.66       |
| (1,845)  | 1:A:147:GLY:HA2  | 1:A:133:ILE:HD11 | 2                   | 0.66     | 0.09                | 0.66       |
| (1,845)  | 1:A:147:GLY:HA2  | 1:A:133:ILE:HD12 | 2                   | 0.66     | 0.09                | 0.66       |
| (1,845)  | 1:A:147:GLY:HA2  | 1:A:133:ILE:HD13 | 2                   | 0.66     | 0.09                | 0.66       |
| (1,1739) | 1:A:111:HIS:HA   | 1:B:122:TYR:HE1  | 2                   | 0.59     | 0.21                | 0.59       |
| (1,1739) | 1:A:111:HIS:HA   | 1:B:122:TYR:HE2  | 2                   | 0.59     | 0.21                | 0.59       |
| (1,1749) | 1:A:115:SER:HB3  | 1:B:119:HIS:HE1  | 2                   | 0.57     | 0.35                | 0.57       |
| (1,200)  | 1:A:84:PHE:HD1   | 1:A:85:SER:H     | 2                   | 0.56     | 0.2                 | 0.56       |
| (1,200)  | 1:A:84:PHE:HD2   | 1:A:85:SER:H     | 2                   | 0.56     | 0.2                 | 0.56       |
| (1,547)  | 1:A:117:GLU:H    | 1:A:117:GLU:HG2  | 2                   | 0.56     | 0.12                | 0.56       |
| (1,547)  | 1:A:117:GLU:H    | 1:A:117:GLU:HG3  | 2                   | 0.56     | 0.12                | 0.56       |
| (1,1067) | 1:B:84:PHE:HD1   | 1:B:85:SER:H     | 2                   | 0.56     | 0.2                 | 0.56       |
| (1,1067) | 1:B:84:PHE:HD2   | 1:B:85:SER:H     | 2                   | 0.56     | 0.2                 | 0.56       |
| (1,1414) | 1:B:117:GLU:H    | 1:B:117:GLU:HG2  | 2                   | 0.56     | 0.12                | 0.56       |
| (1,1414) | 1:B:117:GLU:H    | 1:B:117:GLU:HG3  | 2                   | 0.56     | 0.12                | 0.56       |
| (1,171)  | 1:A:83:HIS:H     | 1:A:82:LYS:HG2   | 2                   | 0.52     | 0.05                | 0.52       |
| (1,171)  | 1:A:83:HIS:H     | 1:A:82:LYS:HG3   | 2                   | 0.52     | 0.05                | 0.52       |
| (1,1038) | 1:B:83:HIS:H     | 1:B:82:LYS:HG2   | 2                   | 0.52     | 0.05                | 0.52       |
| (1,1038) | 1:B:83:HIS:H     | 1:B:82:LYS:HG3   | 2                   | 0.52     | 0.05                | 0.52       |
| (1,1738) | 1:A:111:HIS:HA   | 1:B:122:TYR:HD1  | 2                   | 0.5      | 0.15                | 0.5        |
| (1,1738) | 1:A:111:HIS:HA   | 1:B:122:TYR:HD2  | 2                   | 0.5      | 0.15                | 0.5        |
| (1,172)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB2   | 2                   | 0.49     | 0.02                | 0.49       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,177)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB2  | 2                   | 0.49     | 0.02                | 0.49       |
| (1,1039) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB2  | 2                   | 0.49     | 0.02                | 0.49       |
| (1,1044) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB2  | 2                   | 0.49     | 0.02                | 0.49       |
| (1,592)  | 1:A:122:TYR:HA   | 1:A:122:TYR:HD1 | 2                   | 0.47     | 0.23                | 0.47       |
| (1,592)  | 1:A:122:TYR:HA   | 1:A:122:TYR:HD2 | 2                   | 0.47     | 0.23                | 0.47       |
| (1,1459) | 1:B:122:TYR:HA   | 1:B:122:TYR:HD1 | 2                   | 0.47     | 0.23                | 0.47       |
| (1,1459) | 1:B:122:TYR:HA   | 1:B:122:TYR:HD2 | 2                   | 0.47     | 0.23                | 0.47       |
| (1,179)  | 1:A:83:HIS:HA    | 1:A:83:HIS:H    | 2                   | 0.46     | 0.0                 | 0.46       |
| (1,1046) | 1:B:83:HIS:HA    | 1:B:83:HIS:H    | 2                   | 0.46     | 0.0                 | 0.46       |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG11 | 2                   | 0.44     | 0.31                | 0.44       |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG12 | 2                   | 0.44     | 0.31                | 0.44       |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG13 | 2                   | 0.44     | 0.31                | 0.44       |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG21 | 2                   | 0.44     | 0.31                | 0.44       |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG22 | 2                   | 0.44     | 0.31                | 0.44       |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG23 | 2                   | 0.44     | 0.31                | 0.44       |
| (1,828)  | 1:A:146:ASP:H    | 1:A:134:THR:H   | 2                   | 0.44     | 0.16                | 0.44       |
| (1,829)  | 1:A:146:ASP:H    | 1:A:134:THR:H   | 2                   | 0.44     | 0.16                | 0.44       |
| (1,1695) | 1:B:146:ASP:H    | 1:B:134:THR:H   | 2                   | 0.44     | 0.16                | 0.44       |
| (1,1696) | 1:B:146:ASP:H    | 1:B:134:THR:H   | 2                   | 0.44     | 0.16                | 0.44       |
| (1,810)  | 1:A:144:THR:HG21 | 1:A:146:ASP:HB2 | 2                   | 0.43     | 0.18                | 0.43       |
| (1,810)  | 1:A:144:THR:HG22 | 1:A:146:ASP:HB2 | 2                   | 0.43     | 0.18                | 0.43       |
| (1,810)  | 1:A:144:THR:HG23 | 1:A:146:ASP:HB2 | 2                   | 0.43     | 0.18                | 0.43       |
| (1,1677) | 1:B:144:THR:HG21 | 1:B:146:ASP:HB2 | 2                   | 0.43     | 0.18                | 0.43       |
| (1,1677) | 1:B:144:THR:HG22 | 1:B:146:ASP:HB2 | 2                   | 0.43     | 0.18                | 0.43       |
| (1,1677) | 1:B:144:THR:HG23 | 1:B:146:ASP:HB2 | 2                   | 0.43     | 0.18                | 0.43       |
| (1,81)   | 1:A:77:VAL:HG11  | 1:A:68:MET:HE1  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,81)   | 1:A:77:VAL:HG11  | 1:A:68:MET:HE2  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,81)   | 1:A:77:VAL:HG11  | 1:A:68:MET:HE3  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,81)   | 1:A:77:VAL:HG12  | 1:A:68:MET:HE1  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,81)   | 1:A:77:VAL:HG12  | 1:A:68:MET:HE2  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,81)   | 1:A:77:VAL:HG12  | 1:A:68:MET:HE3  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,81)   | 1:A:77:VAL:HG13  | 1:A:68:MET:HE1  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,81)   | 1:A:77:VAL:HG13  | 1:A:68:MET:HE2  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,81)   | 1:A:77:VAL:HG13  | 1:A:68:MET:HE3  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,948)  | 1:B:77:VAL:HG11  | 1:B:68:MET:HE1  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,948)  | 1:B:77:VAL:HG11  | 1:B:68:MET:HE2  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,948)  | 1:B:77:VAL:HG11  | 1:B:68:MET:HE3  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,948)  | 1:B:77:VAL:HG12  | 1:B:68:MET:HE1  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,948)  | 1:B:77:VAL:HG12  | 1:B:68:MET:HE2  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,948)  | 1:B:77:VAL:HG12  | 1:B:68:MET:HE3  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,948)  | 1:B:77:VAL:HG13  | 1:B:68:MET:HE1  | 2                   | 0.4      | 0.08                | 0.4        |
| (1,948)  | 1:B:77:VAL:HG13  | 1:B:68:MET:HE2  | 2                   | 0.4      | 0.08                | 0.4        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,948)  | 1:B:77:VAL:HG13  | 1:B:68:MET:HE3   | 2                   | 0.4      | 0.08                | 0.4        |
| (1,1553) | 1:B:129:ASP:H    | 1:B:132:THR:HG1  | 2                   | 0.4      | 0.14                | 0.4        |
| (1,580)  | 1:A:120:ARG:H    | 1:A:100:VAL:H    | 2                   | 0.39     | 0.18                | 0.39       |
| (1,713)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HB2  | 2                   | 0.39     | 0.28                | 0.39       |
| (1,713)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HB3  | 2                   | 0.39     | 0.28                | 0.39       |
| (1,713)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HB2  | 2                   | 0.39     | 0.28                | 0.39       |
| (1,713)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HB3  | 2                   | 0.39     | 0.28                | 0.39       |
| (1,713)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HB2  | 2                   | 0.39     | 0.28                | 0.39       |
| (1,713)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HB3  | 2                   | 0.39     | 0.28                | 0.39       |
| (1,1447) | 1:B:120:ARG:H    | 1:B:100:VAL:H    | 2                   | 0.39     | 0.17                | 0.39       |
| (1,320)  | 1:A:96:ASP:HA    | 1:A:124:ILE:H    | 2                   | 0.38     | 0.14                | 0.38       |
| (1,1187) | 1:B:96:ASP:HA    | 1:B:124:ILE:H    | 2                   | 0.38     | 0.14                | 0.38       |
| (1,137)  | 1:A:79:LEU:HA    | 1:A:79:LEU:HG    | 2                   | 0.37     | 0.0                 | 0.37       |
| (1,1004) | 1:B:79:LEU:HA    | 1:B:79:LEU:HG    | 2                   | 0.37     | 0.0                 | 0.37       |
| (1,113)  | 1:A:77:VAL:HB    | 1:A:145:VAL:HG21 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,113)  | 1:A:77:VAL:HB    | 1:A:145:VAL:HG22 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,113)  | 1:A:77:VAL:HB    | 1:A:145:VAL:HG23 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,715)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HG2  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,715)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HG3  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,715)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HG2  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,715)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HG3  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,715)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HG2  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,715)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HG3  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,980)  | 1:B:77:VAL:HB    | 1:B:145:VAL:HG21 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,980)  | 1:B:77:VAL:HB    | 1:B:145:VAL:HG22 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,980)  | 1:B:77:VAL:HB    | 1:B:145:VAL:HG23 | 2                   | 0.36     | 0.05                | 0.36       |
| (1,1043) | 1:B:83:HIS:HB3   | 1:B:83:HIS:HD2   | 2                   | 0.36     | 0.16                | 0.36       |
| (1,1582) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HG2  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,1582) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HG3  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,1582) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HG2  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,1582) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HG3  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,1582) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HG2  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,1582) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HG3  | 2                   | 0.36     | 0.12                | 0.36       |
| (1,8)    | 1:A:68:MET:HG2   | 1:A:68:MET:H     | 2                   | 0.34     | 0.13                | 0.34       |
| (1,8)    | 1:A:68:MET:HG3   | 1:A:68:MET:H     | 2                   | 0.34     | 0.13                | 0.34       |
| (1,875)  | 1:B:68:MET:HG2   | 1:B:68:MET:H     | 2                   | 0.34     | 0.13                | 0.34       |
| (1,875)  | 1:B:68:MET:HG3   | 1:B:68:MET:H     | 2                   | 0.34     | 0.13                | 0.34       |
| (1,404)  | 1:A:104:HIS:HB3  | 1:A:104:HIS:HA   | 2                   | 0.34     | 0.08                | 0.34       |
| (1,405)  | 1:A:104:HIS:HB3  | 1:A:104:HIS:HA   | 2                   | 0.34     | 0.08                | 0.34       |
| (1,1271) | 1:B:104:HIS:HB3  | 1:B:104:HIS:HA   | 2                   | 0.34     | 0.08                | 0.34       |
| (1,1272) | 1:B:104:HIS:HB3  | 1:B:104:HIS:HA   | 2                   | 0.34     | 0.08                | 0.34       |
| (1,464)  | 1:A:111:HIS:H    | 1:A:111:HIS:HD2  | 2                   | 0.34     | 0.13                | 0.34       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,59)   | 1:A:76:SER:HB2   | 1:A:75:PHE:HD1   | 2                   | 0.33     | 0.18                | 0.33       |
| (1,59)   | 1:A:76:SER:HB2   | 1:A:75:PHE:HD2   | 2                   | 0.33     | 0.18                | 0.33       |
| (1,926)  | 1:B:76:SER:HB2   | 1:B:75:PHE:HD1   | 2                   | 0.33     | 0.18                | 0.33       |
| (1,926)  | 1:B:76:SER:HB2   | 1:B:75:PHE:HD2   | 2                   | 0.33     | 0.18                | 0.33       |
| (1,189)  | 1:A:84:PHE:H     | 1:A:81:VAL:HB    | 2                   | 0.32     | 0.09                | 0.32       |
| (1,553)  | 1:A:118:PHE:HD1  | 1:A:103:LYS:H    | 2                   | 0.32     | 0.18                | 0.32       |
| (1,553)  | 1:A:118:PHE:HD2  | 1:A:103:LYS:H    | 2                   | 0.32     | 0.18                | 0.32       |
| (1,1056) | 1:B:84:PHE:H     | 1:B:81:VAL:HB    | 2                   | 0.32     | 0.09                | 0.32       |
| (1,1420) | 1:B:118:PHE:HD1  | 1:B:103:LYS:H    | 2                   | 0.32     | 0.19                | 0.32       |
| (1,1420) | 1:B:118:PHE:HD2  | 1:B:103:LYS:H    | 2                   | 0.32     | 0.19                | 0.32       |
| (1,176)  | 1:A:83:HIS:HB3   | 1:A:83:HIS:HD2   | 2                   | 0.32     | 0.12                | 0.32       |
| (1,1580) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HB2  | 2                   | 0.3      | 0.2                 | 0.3        |
| (1,1580) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HB3  | 2                   | 0.3      | 0.2                 | 0.3        |
| (1,1580) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HB2  | 2                   | 0.3      | 0.2                 | 0.3        |
| (1,1580) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HB3  | 2                   | 0.3      | 0.2                 | 0.3        |
| (1,1580) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HB2  | 2                   | 0.3      | 0.2                 | 0.3        |
| (1,1580) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HB3  | 2                   | 0.3      | 0.2                 | 0.3        |
| (1,729)  | 1:A:134:THR:H    | 1:A:134:THR:HG21 | 2                   | 0.3      | 0.03                | 0.3        |
| (1,729)  | 1:A:134:THR:H    | 1:A:134:THR:HG22 | 2                   | 0.3      | 0.03                | 0.3        |
| (1,729)  | 1:A:134:THR:H    | 1:A:134:THR:HG23 | 2                   | 0.3      | 0.03                | 0.3        |
| (1,392)  | 1:A:102:GLY:H    | 1:A:118:PHE:H    | 2                   | 0.28     | 0.08                | 0.28       |
| (1,1259) | 1:B:102:GLY:H    | 1:B:118:PHE:H    | 2                   | 0.28     | 0.08                | 0.28       |
| (1,1596) | 1:B:134:THR:H    | 1:B:134:THR:HG21 | 2                   | 0.28     | 0.02                | 0.28       |
| (1,1596) | 1:B:134:THR:H    | 1:B:134:THR:HG22 | 2                   | 0.28     | 0.02                | 0.28       |
| (1,1596) | 1:B:134:THR:H    | 1:B:134:THR:HG23 | 2                   | 0.28     | 0.02                | 0.28       |
| (1,399)  | 1:A:103:LYS:HA   | 1:A:118:PHE:H    | 2                   | 0.26     | 0.03                | 0.26       |
| (1,1266) | 1:B:103:LYS:HA   | 1:B:118:PHE:H    | 2                   | 0.26     | 0.03                | 0.26       |
| (1,292)  | 1:A:94:LEU:HD11  | 1:A:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,292)  | 1:A:94:LEU:HD12  | 1:A:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,292)  | 1:A:94:LEU:HD13  | 1:A:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,292)  | 1:A:94:LEU:HD21  | 1:A:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,292)  | 1:A:94:LEU:HD22  | 1:A:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,292)  | 1:A:94:LEU:HD23  | 1:A:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,1159) | 1:B:94:LEU:HD11  | 1:B:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,1159) | 1:B:94:LEU:HD12  | 1:B:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,1159) | 1:B:94:LEU:HD13  | 1:B:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,1159) | 1:B:94:LEU:HD21  | 1:B:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,1159) | 1:B:94:LEU:HD22  | 1:B:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,1159) | 1:B:94:LEU:HD23  | 1:B:95:GLY:H     | 2                   | 0.24     | 0.03                | 0.24       |
| (1,164)  | 1:A:81:VAL:HG21  | 1:A:84:PHE:H     | 2                   | 0.24     | 0.04                | 0.24       |
| (1,164)  | 1:A:81:VAL:HG22  | 1:A:84:PHE:H     | 2                   | 0.24     | 0.04                | 0.24       |
| (1,164)  | 1:A:81:VAL:HG23  | 1:A:84:PHE:H     | 2                   | 0.24     | 0.04                | 0.24       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1031) | 1:B:81:VAL:HG21 | 1:B:84:PHE:H    | 2                   | 0.24     | 0.04                | 0.24       |
| (1,1031) | 1:B:81:VAL:HG22 | 1:B:84:PHE:H    | 2                   | 0.24     | 0.04                | 0.24       |
| (1,1031) | 1:B:81:VAL:HG23 | 1:B:84:PHE:H    | 2                   | 0.24     | 0.04                | 0.24       |
| (1,838)  | 1:A:146:ASP:HB3 | 1:A:146:ASP:H   | 2                   | 0.24     | 0.1                 | 0.24       |
| (1,1705) | 1:B:146:ASP:HB3 | 1:B:146:ASP:H   | 2                   | 0.24     | 0.1                 | 0.24       |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD11 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD12 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD13 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD21 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD22 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD23 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD11 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD12 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD13 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD21 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD22 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD23 | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,54)   | 1:A:75:PHE:HD1  | 1:A:146:ASP:HB3 | 2                   | 0.23     | 0.05                | 0.23       |
| (1,54)   | 1:A:75:PHE:HD2  | 1:A:146:ASP:HB3 | 2                   | 0.23     | 0.05                | 0.23       |
| (1,921)  | 1:B:75:PHE:HD1  | 1:B:146:ASP:HB3 | 2                   | 0.23     | 0.05                | 0.23       |
| (1,921)  | 1:B:75:PHE:HD2  | 1:B:146:ASP:HB3 | 2                   | 0.23     | 0.05                | 0.23       |
| (1,777)  | 1:A:142:VAL:H   | 1:A:141:GLY:H   | 2                   | 0.23     | 0.08                | 0.23       |
| (1,778)  | 1:A:142:VAL:H   | 1:A:141:GLY:H   | 2                   | 0.23     | 0.08                | 0.23       |
| (1,21)   | 1:A:70:LEU:HD11 | 1:A:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,21)   | 1:A:70:LEU:HD12 | 1:A:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,21)   | 1:A:70:LEU:HD13 | 1:A:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,21)   | 1:A:70:LEU:HD21 | 1:A:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,21)   | 1:A:70:LEU:HD22 | 1:A:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,21)   | 1:A:70:LEU:HD23 | 1:A:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD11 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD12 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD13 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD21 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD22 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD23 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,888)  | 1:B:70:LEU:HD11 | 1:B:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,888)  | 1:B:70:LEU:HD12 | 1:B:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,888)  | 1:B:70:LEU:HD13 | 1:B:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,888)  | 1:B:70:LEU:HD21 | 1:B:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,888)  | 1:B:70:LEU:HD22 | 1:B:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,888)  | 1:B:70:LEU:HD23 | 1:B:71:GLU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,1644) | 1:B:142:VAL:H   | 1:B:141:GLY:H   | 2                   | 0.22     | 0.08                | 0.22       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1645) | 1:B:142:VAL:H    | 1:B:141:GLY:H   | 2                   | 0.22     | 0.08                | 0.22       |
| (1,1760) | 1:A:138:SER:H    | 1:A:142:VAL:H   | 2                   | 0.22     | 0.08                | 0.22       |
| (1,1763) | 1:A:138:SER:H    | 1:A:142:VAL:H   | 2                   | 0.22     | 0.08                | 0.22       |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD11 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD12 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD13 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD21 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD22 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD23 | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1627) | 1:B:138:SER:H    | 1:B:142:VAL:H   | 2                   | 0.22     | 0.08                | 0.22       |
| (1,1630) | 1:B:138:SER:H    | 1:B:142:VAL:H   | 2                   | 0.22     | 0.08                | 0.22       |
| (1,1528) | 1:B:126:ALA:HB1  | 1:B:128:VAL:H   | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,1528) | 1:B:126:ALA:HB2  | 1:B:128:VAL:H   | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,1528) | 1:B:126:ALA:HB3  | 1:B:128:VAL:H   | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,785)  | 1:A:142:VAL:HG11 | 1:A:143:LEU:H   | 2                   | 0.21     | 0.05                | 0.21       |
| (1,785)  | 1:A:142:VAL:HG12 | 1:A:143:LEU:H   | 2                   | 0.21     | 0.05                | 0.21       |
| (1,785)  | 1:A:142:VAL:HG13 | 1:A:143:LEU:H   | 2                   | 0.21     | 0.05                | 0.21       |
| (1,785)  | 1:A:142:VAL:HG21 | 1:A:143:LEU:H   | 2                   | 0.21     | 0.05                | 0.21       |
| (1,785)  | 1:A:142:VAL:HG22 | 1:A:143:LEU:H   | 2                   | 0.21     | 0.05                | 0.21       |
| (1,785)  | 1:A:142:VAL:HG23 | 1:A:143:LEU:H   | 2                   | 0.21     | 0.05                | 0.21       |
| (1,661)  | 1:A:126:ALA:HB1  | 1:A:128:VAL:H   | 2                   | 0.21     | 0.1                 | 0.21       |
| (1,661)  | 1:A:126:ALA:HB2  | 1:A:128:VAL:H   | 2                   | 0.21     | 0.1                 | 0.21       |
| (1,661)  | 1:A:126:ALA:HB3  | 1:A:128:VAL:H   | 2                   | 0.21     | 0.1                 | 0.21       |
| (1,705)  | 1:A:132:THR:HG1  | 1:A:133:ILE:H   | 2                   | 0.2      | 0.03                | 0.2        |
| (1,1652) | 1:B:142:VAL:HG11 | 1:B:143:LEU:H   | 2                   | 0.2      | 0.06                | 0.2        |
| (1,1652) | 1:B:142:VAL:HG12 | 1:B:143:LEU:H   | 2                   | 0.2      | 0.06                | 0.2        |
| (1,1652) | 1:B:142:VAL:HG13 | 1:B:143:LEU:H   | 2                   | 0.2      | 0.06                | 0.2        |
| (1,1652) | 1:B:142:VAL:HG21 | 1:B:143:LEU:H   | 2                   | 0.2      | 0.06                | 0.2        |
| (1,1652) | 1:B:142:VAL:HG22 | 1:B:143:LEU:H   | 2                   | 0.2      | 0.06                | 0.2        |
| (1,1652) | 1:B:142:VAL:HG23 | 1:B:143:LEU:H   | 2                   | 0.2      | 0.06                | 0.2        |
| (1,168)  | 1:A:81:VAL:HG21  | 1:A:143:LEU:HA  | 2                   | 0.2      | 0.03                | 0.2        |
| (1,168)  | 1:A:81:VAL:HG22  | 1:A:143:LEU:HA  | 2                   | 0.2      | 0.03                | 0.2        |
| (1,168)  | 1:A:81:VAL:HG23  | 1:A:143:LEU:HA  | 2                   | 0.2      | 0.03                | 0.2        |
| (1,419)  | 1:A:105:GLU:HA   | 1:A:116:ARG:H   | 2                   | 0.2      | 0.08                | 0.2        |
| (1,1035) | 1:B:81:VAL:HG21  | 1:B:143:LEU:HA  | 2                   | 0.2      | 0.03                | 0.2        |
| (1,1035) | 1:B:81:VAL:HG22  | 1:B:143:LEU:HA  | 2                   | 0.2      | 0.03                | 0.2        |
| (1,1035) | 1:B:81:VAL:HG23  | 1:B:143:LEU:HA  | 2                   | 0.2      | 0.03                | 0.2        |
| (1,1286) | 1:B:105:GLU:HA   | 1:B:116:ARG:H   | 2                   | 0.2      | 0.08                | 0.2        |
| (1,675)  | 1:A:128:VAL:H    | 1:A:126:ALA:H   | 2                   | 0.2      | 0.04                | 0.2        |
| (1,1542) | 1:B:128:VAL:H    | 1:B:126:ALA:H   | 2                   | 0.2      | 0.04                | 0.2        |
| (1,1661) | 1:B:144:THR:HG21 | 1:B:78:ASN:HA   | 2                   | 0.18     | 0.01                | 0.18       |
| (1,1661) | 1:B:144:THR:HG22 | 1:B:78:ASN:HA   | 2                   | 0.18     | 0.01                | 0.18       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1661) | 1:B:144:THR:HG23 | 1:B:78:ASN:HA   | 2                   | 0.18     | 0.01                | 0.18       |
| (1,293)  | 1:A:94:LEU:H     | 1:A:95:GLY:H    | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1160) | 1:B:94:LEU:H     | 1:B:95:GLY:H    | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1744) | 1:A:114:ILE:HA   | 1:B:120:ARG:HB2 | 2                   | 0.17     | 0.05                | 0.17       |
| (1,1744) | 1:A:114:ILE:HA   | 1:B:120:ARG:HB3 | 2                   | 0.17     | 0.05                | 0.17       |
| (1,533)  | 1:A:115:SER:HB2  | 1:A:116:ARG:H   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1400) | 1:B:115:SER:HB2  | 1:B:116:ARG:H   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1045) | 1:B:83:HIS:HB3   | 1:B:83:HIS:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1572) | 1:B:132:THR:HG1  | 1:B:133:ILE:H   | 2                   | 0.16     | 0.05                | 0.16       |
| (1,178)  | 1:A:83:HIS:HB3   | 1:A:83:HIS:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,802)  | 1:A:144:THR:HB   | 1:A:144:THR:H   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1669) | 1:B:144:THR:HB   | 1:B:144:THR:H   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,521)  | 1:A:115:SER:HB2  | 1:A:105:GLU:HB2 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,521)  | 1:A:115:SER:HB2  | 1:A:105:GLU:HB3 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1388) | 1:B:115:SER:HB2  | 1:B:105:GLU:HB2 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1388) | 1:B:115:SER:HB2  | 1:B:105:GLU:HB3 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,853)  | 1:A:148:PRO:HA   | 1:A:148:PRO:HG2 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,853)  | 1:A:148:PRO:HA   | 1:A:148:PRO:HG3 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,1720) | 1:B:148:PRO:HA   | 1:B:148:PRO:HG2 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,1720) | 1:B:148:PRO:HA   | 1:B:148:PRO:HG3 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,541)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HG2 | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,541)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HG3 | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,542)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HD2 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,542)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HD3 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,737)  | 1:A:135:SER:HA   | 1:A:136:SER:H   | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1408) | 1:B:117:GLU:HA   | 1:B:103:LYS:HG2 | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,1408) | 1:B:117:GLU:HA   | 1:B:103:LYS:HG3 | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,1409) | 1:B:117:GLU:HA   | 1:B:103:LYS:HD2 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1409) | 1:B:117:GLU:HA   | 1:B:103:LYS:HD3 | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1604) | 1:B:135:SER:HA   | 1:B:136:SER:H   | 2                   | 0.13     | 0.02                | 0.13       |

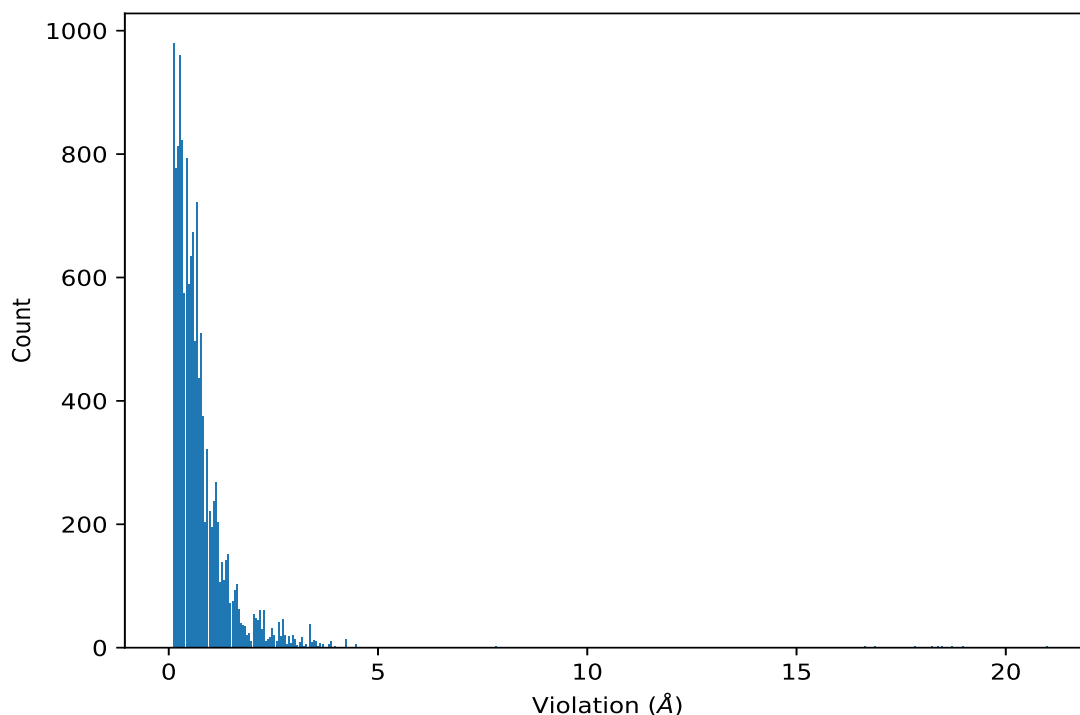
<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 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) |
|----------|-----------------|---------------|----------|---------------|
| (1,1769) | 1:A:122:TYR:HD1 | 1:B:121:LYS:H | 2        | 20.97         |
| (1,1769) | 1:A:122:TYR:HD2 | 1:B:121:LYS:H | 2        | 20.97         |
| (1,1769) | 1:A:122:TYR:HD1 | 1:B:121:LYS:H | 7        | 18.97         |
| (1,1769) | 1:A:122:TYR:HD2 | 1:B:121:LYS:H | 7        | 18.97         |
| (1,1769) | 1:A:122:TYR:HD1 | 1:B:121:LYS:H | 3        | 18.73         |
| (1,1769) | 1:A:122:TYR:HD2 | 1:B:121:LYS:H | 3        | 18.73         |
| (1,1769) | 1:A:122:TYR:HD1 | 1:B:121:LYS:H | 8        | 18.48         |
| (1,1769) | 1:A:122:TYR:HD2 | 1:B:121:LYS:H | 8        | 18.48         |
| (1,1769) | 1:A:122:TYR:HD1 | 1:B:121:LYS:H | 1        | 18.39         |
| (1,1769) | 1:A:122:TYR:HD2 | 1:B:121:LYS:H | 1        | 18.39         |
| (1,1769) | 1:A:122:TYR:HD1 | 1:B:121:LYS:H | 4        | 18.24         |
| (1,1769) | 1:A:122:TYR:HD2 | 1:B:121:LYS:H | 4        | 18.24         |
| (1,1769) | 1:A:122:TYR:HD1 | 1:B:121:LYS:H | 9        | 17.84         |
| (1,1769) | 1:A:122:TYR:HD2 | 1:B:121:LYS:H | 9        | 17.84         |
| (1,1769) | 1:A:122:TYR:HD1 | 1:B:121:LYS:H | 6        | 16.85         |
| (1,1769) | 1:A:122:TYR:HD2 | 1:B:121:LYS:H | 6        | 16.85         |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1769) | 1:A:122:TYR:HD1  | 1:B:121:LYS:H    | 5        | 16.6          |
| (1,1769) | 1:A:122:TYR:HD2  | 1:B:121:LYS:H    | 5        | 16.6          |
| (1,1741) | 1:A:114:ILE:HA   | 1:B:116:ARG:HA   | 5        | 8.53          |
| (1,1741) | 1:A:114:ILE:HA   | 1:B:116:ARG:HA   | 8        | 7.99          |
| (1,1741) | 1:A:114:ILE:HA   | 1:B:116:ARG:HA   | 6        | 7.81          |
| (1,1741) | 1:A:114:ILE:HA   | 1:B:116:ARG:HA   | 7        | 7.81          |
| (1,1741) | 1:A:114:ILE:HA   | 1:B:116:ARG:HA   | 4        | 7.47          |
| (1,1741) | 1:A:114:ILE:HA   | 1:B:116:ARG:HA   | 2        | 7.44          |
| (1,1741) | 1:A:114:ILE:HA   | 1:B:116:ARG:HA   | 9        | 7.31          |
| (1,1741) | 1:A:114:ILE:HA   | 1:B:116:ARG:HA   | 3        | 7.21          |
| (1,1741) | 1:A:114:ILE:HA   | 1:B:116:ARG:HA   | 1        | 6.48          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD1  | 8        | 4.46          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD2  | 8        | 4.46          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD1  | 8        | 4.46          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD2  | 8        | 4.46          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD1  | 8        | 4.46          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD2  | 8        | 4.46          |
| (1,1754) | 1:A:118:PHE:HZ   | 1:B:116:ARG:HA   | 4        | 4.28          |
| (1,1754) | 1:A:118:PHE:HZ   | 1:B:116:ARG:HA   | 7        | 4.23          |
| (1,641)  | 1:A:124:ILE:HG21 | 1:A:148:PRO:HA   | 2        | 4.21          |
| (1,641)  | 1:A:124:ILE:HG22 | 1:A:148:PRO:HA   | 2        | 4.21          |
| (1,641)  | 1:A:124:ILE:HG23 | 1:A:148:PRO:HA   | 2        | 4.21          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG21 | 7        | 4.21          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG22 | 7        | 4.21          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG23 | 7        | 4.21          |
| (1,1508) | 1:B:124:ILE:HG21 | 1:B:148:PRO:HA   | 2        | 4.21          |
| (1,1508) | 1:B:124:ILE:HG22 | 1:B:148:PRO:HA   | 2        | 4.21          |
| (1,1508) | 1:B:124:ILE:HG23 | 1:B:148:PRO:HA   | 2        | 4.21          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG21 | 7        | 4.21          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG22 | 7        | 4.21          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG23 | 7        | 4.21          |
| (1,1761) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H    | 5        | 3.98          |
| (1,1761) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H    | 5        | 3.98          |
| (1,1754) | 1:A:118:PHE:HZ   | 1:B:116:ARG:HA   | 5        | 3.97          |
| (1,520)  | 1:A:115:SER:HA   | 1:A:104:HIS:HE1  | 3        | 3.9           |
| (1,1387) | 1:B:115:SER:HA   | 1:B:104:HIS:HE1  | 3        | 3.9           |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD1  | 2        | 3.86          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD2  | 2        | 3.86          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD1  | 2        | 3.86          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD2  | 2        | 3.86          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD1  | 2        | 3.86          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD2  | 2        | 3.86          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,321)  | 1:A:97:VAL:H     | 1:A:93:VAL:HB    | 8        | 3.85          |
| (1,1188) | 1:B:97:VAL:H     | 1:B:93:VAL:HB    | 8        | 3.85          |
| (1,357)  | 1:A:100:VAL:HG11 | 1:A:80:ASP:HA    | 9        | 3.81          |
| (1,357)  | 1:A:100:VAL:HG12 | 1:A:80:ASP:HA    | 9        | 3.81          |
| (1,357)  | 1:A:100:VAL:HG13 | 1:A:80:ASP:HA    | 9        | 3.81          |
| (1,1224) | 1:B:100:VAL:HG11 | 1:B:80:ASP:HA    | 9        | 3.81          |
| (1,1224) | 1:B:100:VAL:HG12 | 1:B:80:ASP:HA    | 9        | 3.81          |
| (1,1224) | 1:B:100:VAL:HG13 | 1:B:80:ASP:HA    | 9        | 3.81          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG21 | 4        | 3.69          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG22 | 4        | 3.69          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG23 | 4        | 3.69          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG21 | 4        | 3.68          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG22 | 4        | 3.68          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG23 | 4        | 3.68          |
| (1,357)  | 1:A:100:VAL:HG11 | 1:A:80:ASP:HA    | 5        | 3.62          |
| (1,357)  | 1:A:100:VAL:HG12 | 1:A:80:ASP:HA    | 5        | 3.62          |
| (1,357)  | 1:A:100:VAL:HG13 | 1:A:80:ASP:HA    | 5        | 3.62          |
| (1,1224) | 1:B:100:VAL:HG11 | 1:B:80:ASP:HA    | 5        | 3.62          |
| (1,1224) | 1:B:100:VAL:HG12 | 1:B:80:ASP:HA    | 5        | 3.62          |
| (1,1224) | 1:B:100:VAL:HG13 | 1:B:80:ASP:HA    | 5        | 3.62          |
| (1,321)  | 1:A:97:VAL:H     | 1:A:93:VAL:HB    | 2        | 3.61          |
| (1,1188) | 1:B:97:VAL:H     | 1:B:93:VAL:HB    | 2        | 3.61          |
| (1,1761) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H    | 7        | 3.57          |
| (1,1761) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H    | 7        | 3.57          |
| (1,520)  | 1:A:115:SER:HA   | 1:A:104:HIS:HE1  | 6        | 3.55          |
| (1,434)  | 1:A:107:ARG:HD3  | 1:A:109:ASP:H    | 7        | 3.55          |
| (1,1387) | 1:B:115:SER:HA   | 1:B:104:HIS:HE1  | 6        | 3.55          |
| (1,1301) | 1:B:107:ARG:HD3  | 1:B:109:ASP:H    | 7        | 3.55          |
| (1,151)  | 1:A:81:VAL:HG11  | 1:A:79:LEU:HG    | 4        | 3.5           |
| (1,151)  | 1:A:81:VAL:HG12  | 1:A:79:LEU:HG    | 4        | 3.5           |
| (1,151)  | 1:A:81:VAL:HG13  | 1:A:79:LEU:HG    | 4        | 3.5           |
| (1,1018) | 1:B:81:VAL:HG11  | 1:B:79:LEU:HG    | 4        | 3.5           |
| (1,1018) | 1:B:81:VAL:HG12  | 1:B:79:LEU:HG    | 4        | 3.5           |
| (1,1018) | 1:B:81:VAL:HG13  | 1:B:79:LEU:HG    | 4        | 3.5           |
| (1,1224) | 1:B:100:VAL:HG11 | 1:B:80:ASP:HA    | 6        | 3.48          |
| (1,1224) | 1:B:100:VAL:HG12 | 1:B:80:ASP:HA    | 6        | 3.48          |
| (1,1224) | 1:B:100:VAL:HG13 | 1:B:80:ASP:HA    | 6        | 3.48          |
| (1,357)  | 1:A:100:VAL:HG11 | 1:A:80:ASP:HA    | 6        | 3.47          |
| (1,357)  | 1:A:100:VAL:HG12 | 1:A:80:ASP:HA    | 6        | 3.47          |
| (1,357)  | 1:A:100:VAL:HG13 | 1:A:80:ASP:HA    | 6        | 3.47          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG21 | 2        | 3.45          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG22 | 2        | 3.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG23 | 2        | 3.45          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG21 | 2        | 3.45          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG22 | 2        | 3.45          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG23 | 2        | 3.45          |
| (1,436)  | 1:A:107:ARG:HB2  | 1:A:109:ASP:H    | 1        | 3.43          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD1  | 7        | 3.43          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD2  | 7        | 3.43          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD1  | 7        | 3.43          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD2  | 7        | 3.43          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD1  | 7        | 3.43          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD2  | 7        | 3.43          |
| (1,1303) | 1:B:107:ARG:HB2  | 1:B:109:ASP:H    | 1        | 3.43          |
| (1,1754) | 1:A:118:PHE:HZ   | 1:B:116:ARG:HA   | 9        | 3.42          |
| (1,357)  | 1:A:100:VAL:HG11 | 1:A:80:ASP:HA    | 2        | 3.38          |
| (1,357)  | 1:A:100:VAL:HG12 | 1:A:80:ASP:HA    | 2        | 3.38          |
| (1,357)  | 1:A:100:VAL:HG13 | 1:A:80:ASP:HA    | 2        | 3.38          |
| (1,1224) | 1:B:100:VAL:HG11 | 1:B:80:ASP:HA    | 2        | 3.38          |
| (1,1224) | 1:B:100:VAL:HG12 | 1:B:80:ASP:HA    | 2        | 3.38          |
| (1,1224) | 1:B:100:VAL:HG13 | 1:B:80:ASP:HA    | 2        | 3.38          |
| (1,357)  | 1:A:100:VAL:HG11 | 1:A:80:ASP:HA    | 1        | 3.37          |
| (1,357)  | 1:A:100:VAL:HG12 | 1:A:80:ASP:HA    | 1        | 3.37          |
| (1,357)  | 1:A:100:VAL:HG13 | 1:A:80:ASP:HA    | 1        | 3.37          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD1  | 3        | 3.37          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD2  | 3        | 3.37          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD1  | 3        | 3.37          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD2  | 3        | 3.37          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD1  | 3        | 3.37          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD2  | 3        | 3.37          |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD1  | 8        | 3.37          |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD2  | 8        | 3.37          |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD1  | 8        | 3.37          |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD2  | 8        | 3.37          |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD1  | 8        | 3.37          |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD2  | 8        | 3.37          |
| (1,1224) | 1:B:100:VAL:HG11 | 1:B:80:ASP:HA    | 1        | 3.37          |
| (1,1224) | 1:B:100:VAL:HG12 | 1:B:80:ASP:HA    | 1        | 3.37          |
| (1,1224) | 1:B:100:VAL:HG13 | 1:B:80:ASP:HA    | 1        | 3.37          |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD1  | 8        | 3.37          |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD2  | 8        | 3.37          |
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD1  | 8        | 3.37          |
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD2  | 8        | 3.37          |
| (1,1032) | 1:B:81:VAL:HG23  | 1:B:118:PHE:HD1  | 8        | 3.37          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1032) | 1:B:81:VAL:HG23 | 1:B:118:PHE:HD2  | 8        | 3.37          |
| (1,1760) | 1:A:120:ARG:HB2 | 1:B:111:HIS:H    | 5        | 3.35          |
| (1,1760) | 1:A:120:ARG:HB3 | 1:B:111:HIS:H    | 5        | 3.35          |
| (1,151)  | 1:A:81:VAL:HG11 | 1:A:79:LEU:HG    | 7        | 3.35          |
| (1,151)  | 1:A:81:VAL:HG12 | 1:A:79:LEU:HG    | 7        | 3.35          |
| (1,151)  | 1:A:81:VAL:HG13 | 1:A:79:LEU:HG    | 7        | 3.35          |
| (1,1018) | 1:B:81:VAL:HG11 | 1:B:79:LEU:HG    | 7        | 3.35          |
| (1,1018) | 1:B:81:VAL:HG12 | 1:B:79:LEU:HG    | 7        | 3.35          |
| (1,1018) | 1:B:81:VAL:HG13 | 1:B:79:LEU:HG    | 7        | 3.35          |
| (1,520)  | 1:A:115:SER:HA  | 1:A:104:HIS:HE1  | 2        | 3.29          |
| (1,1387) | 1:B:115:SER:HA  | 1:B:104:HIS:HE1  | 2        | 3.28          |
| (1,520)  | 1:A:115:SER:HA  | 1:A:104:HIS:HE1  | 9        | 3.27          |
| (1,1387) | 1:B:115:SER:HA  | 1:B:104:HIS:HE1  | 9        | 3.27          |
| (1,1761) | 1:A:120:ARG:HB2 | 1:B:111:HIS:H    | 6        | 3.26          |
| (1,1761) | 1:A:120:ARG:HB3 | 1:B:111:HIS:H    | 6        | 3.26          |
| (1,385)  | 1:A:102:GLY:HA2 | 1:A:84:PHE:HZ    | 4        | 3.22          |
| (1,1252) | 1:B:102:GLY:HA2 | 1:B:84:PHE:HZ    | 4        | 3.22          |
| (1,151)  | 1:A:81:VAL:HG11 | 1:A:79:LEU:HG    | 1        | 3.18          |
| (1,151)  | 1:A:81:VAL:HG12 | 1:A:79:LEU:HG    | 1        | 3.18          |
| (1,151)  | 1:A:81:VAL:HG13 | 1:A:79:LEU:HG    | 1        | 3.18          |
| (1,1416) | 1:B:118:PHE:HB2 | 1:B:100:VAL:HG21 | 9        | 3.18          |
| (1,1416) | 1:B:118:PHE:HB2 | 1:B:100:VAL:HG22 | 9        | 3.18          |
| (1,1416) | 1:B:118:PHE:HB2 | 1:B:100:VAL:HG23 | 9        | 3.18          |
| (1,1018) | 1:B:81:VAL:HG11 | 1:B:79:LEU:HG    | 1        | 3.18          |
| (1,1018) | 1:B:81:VAL:HG12 | 1:B:79:LEU:HG    | 1        | 3.18          |
| (1,1018) | 1:B:81:VAL:HG13 | 1:B:79:LEU:HG    | 1        | 3.18          |
| (1,549)  | 1:A:118:PHE:HB2 | 1:A:100:VAL:HG21 | 9        | 3.17          |
| (1,549)  | 1:A:118:PHE:HB2 | 1:A:100:VAL:HG22 | 9        | 3.17          |
| (1,549)  | 1:A:118:PHE:HB2 | 1:A:100:VAL:HG23 | 9        | 3.17          |
| (1,436)  | 1:A:107:ARG:HB2 | 1:A:109:ASP:H    | 2        | 3.16          |
| (1,1416) | 1:B:118:PHE:HB2 | 1:B:100:VAL:HG21 | 5        | 3.16          |
| (1,1416) | 1:B:118:PHE:HB2 | 1:B:100:VAL:HG22 | 5        | 3.16          |
| (1,1416) | 1:B:118:PHE:HB2 | 1:B:100:VAL:HG23 | 5        | 3.16          |
| (1,1303) | 1:B:107:ARG:HB2 | 1:B:109:ASP:H    | 2        | 3.16          |
| (1,549)  | 1:A:118:PHE:HB2 | 1:A:100:VAL:HG21 | 5        | 3.15          |
| (1,549)  | 1:A:118:PHE:HB2 | 1:A:100:VAL:HG22 | 5        | 3.15          |
| (1,549)  | 1:A:118:PHE:HB2 | 1:A:100:VAL:HG23 | 5        | 3.15          |
| (1,506)  | 1:A:114:ILE:HB  | 1:A:107:ARG:HD3  | 7        | 3.15          |
| (1,1373) | 1:B:114:ILE:HB  | 1:B:107:ARG:HD3  | 7        | 3.15          |
| (1,436)  | 1:A:107:ARG:HB2 | 1:A:109:ASP:H    | 5        | 3.12          |
| (1,1303) | 1:B:107:ARG:HB2 | 1:B:109:ASP:H    | 5        | 3.12          |
| (1,436)  | 1:A:107:ARG:HB2 | 1:A:109:ASP:H    | 7        | 3.1           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1303) | 1:B:107:ARG:HB2  | 1:B:109:ASP:H   | 7        | 3.1           |
| (1,436)  | 1:A:107:ARG:HB2  | 1:A:109:ASP:H   | 6        | 3.09          |
| (1,1303) | 1:B:107:ARG:HB2  | 1:B:109:ASP:H   | 6        | 3.09          |
| (1,436)  | 1:A:107:ARG:HB2  | 1:A:109:ASP:H   | 9        | 3.08          |
| (1,1303) | 1:B:107:ARG:HB2  | 1:B:109:ASP:H   | 9        | 3.08          |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD1 | 6        | 3.04          |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD2 | 6        | 3.04          |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD1 | 6        | 3.04          |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD2 | 6        | 3.04          |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD1 | 6        | 3.04          |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD2 | 6        | 3.04          |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD1 | 6        | 3.04          |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD2 | 6        | 3.04          |
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD1 | 6        | 3.04          |
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD2 | 6        | 3.04          |
| (1,1032) | 1:B:81:VAL:HG23  | 1:B:118:PHE:HD1 | 6        | 3.04          |
| (1,1032) | 1:B:81:VAL:HG23  | 1:B:118:PHE:HD2 | 6        | 3.04          |
| (1,436)  | 1:A:107:ARG:HB2  | 1:A:109:ASP:H   | 8        | 3.0           |
| (1,1303) | 1:B:107:ARG:HB2  | 1:B:109:ASP:H   | 8        | 3.0           |
| (1,357)  | 1:A:100:VAL:HG11 | 1:A:80:ASP:HA   | 7        | 2.99          |
| (1,357)  | 1:A:100:VAL:HG12 | 1:A:80:ASP:HA   | 7        | 2.99          |
| (1,357)  | 1:A:100:VAL:HG13 | 1:A:80:ASP:HA   | 7        | 2.99          |
| (1,1224) | 1:B:100:VAL:HG11 | 1:B:80:ASP:HA   | 7        | 2.99          |
| (1,1224) | 1:B:100:VAL:HG12 | 1:B:80:ASP:HA   | 7        | 2.99          |
| (1,1224) | 1:B:100:VAL:HG13 | 1:B:80:ASP:HA   | 7        | 2.99          |
| (1,357)  | 1:A:100:VAL:HG11 | 1:A:80:ASP:HA   | 4        | 2.96          |
| (1,357)  | 1:A:100:VAL:HG12 | 1:A:80:ASP:HA   | 4        | 2.96          |
| (1,357)  | 1:A:100:VAL:HG13 | 1:A:80:ASP:HA   | 4        | 2.96          |
| (1,1224) | 1:B:100:VAL:HG11 | 1:B:80:ASP:HA   | 4        | 2.96          |
| (1,1224) | 1:B:100:VAL:HG12 | 1:B:80:ASP:HA   | 4        | 2.96          |
| (1,1224) | 1:B:100:VAL:HG13 | 1:B:80:ASP:HA   | 4        | 2.96          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD1  | 9        | 2.95          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD2  | 9        | 2.95          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD1  | 9        | 2.95          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD2  | 9        | 2.95          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD1  | 9        | 2.95          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD2  | 9        | 2.95          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD1  | 9        | 2.95          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD2  | 9        | 2.95          |
| (1,1760) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H   | 7        | 2.94          |
| (1,1760) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H   | 7        | 2.94          |
| (1,357)  | 1:A:100:VAL:HG11 | 1:A:80:ASP:HA   | 8        | 2.91          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,357)  | 1:A:100:VAL:HG12 | 1:A:80:ASP:HA    | 8        | 2.91          |
| (1,357)  | 1:A:100:VAL:HG13 | 1:A:80:ASP:HA    | 8        | 2.91          |
| (1,1224) | 1:B:100:VAL:HG11 | 1:B:80:ASP:HA    | 8        | 2.91          |
| (1,1224) | 1:B:100:VAL:HG12 | 1:B:80:ASP:HA    | 8        | 2.91          |
| (1,1224) | 1:B:100:VAL:HG13 | 1:B:80:ASP:HA    | 8        | 2.91          |
| (1,889)  | 1:B:70:LEU:HB3   | 1:B:74:ARG:H     | 3        | 2.9           |
| (1,22)   | 1:A:70:LEU:HB3   | 1:A:74:ARG:H     | 3        | 2.9           |
| (1,1761) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H    | 1        | 2.9           |
| (1,1761) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H    | 1        | 2.9           |
| (1,1767) | 1:A:122:TYR:HB2  | 1:B:112:GLY:HA3  | 5        | 2.86          |
| (1,1767) | 1:A:122:TYR:HB3  | 1:B:112:GLY:HA3  | 5        | 2.86          |
| (1,1368) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HE1  | 5        | 2.86          |
| (1,1368) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HE1  | 5        | 2.86          |
| (1,1368) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HE1  | 5        | 2.86          |
| (1,501)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HE1  | 5        | 2.85          |
| (1,501)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HE1  | 5        | 2.85          |
| (1,501)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HE1  | 5        | 2.85          |
| (1,254)  | 1:A:89:LEU:HD11  | 1:A:91:VAL:HB    | 3        | 2.85          |
| (1,254)  | 1:A:89:LEU:HD12  | 1:A:91:VAL:HB    | 3        | 2.85          |
| (1,254)  | 1:A:89:LEU:HD13  | 1:A:91:VAL:HB    | 3        | 2.85          |
| (1,1121) | 1:B:89:LEU:HD11  | 1:B:91:VAL:HB    | 3        | 2.85          |
| (1,1121) | 1:B:89:LEU:HD12  | 1:B:91:VAL:HB    | 3        | 2.85          |
| (1,1121) | 1:B:89:LEU:HD13  | 1:B:91:VAL:HB    | 3        | 2.85          |
| (1,434)  | 1:A:107:ARG:HD3  | 1:A:109:ASP:H    | 4        | 2.84          |
| (1,1301) | 1:B:107:ARG:HD3  | 1:B:109:ASP:H    | 4        | 2.84          |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG12 | 3        | 2.83          |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG13 | 3        | 2.83          |
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG12 | 3        | 2.83          |
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG13 | 3        | 2.83          |
| (1,322)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HA    | 5        | 2.8           |
| (1,1189) | 1:B:97:VAL:HB    | 1:B:94:LEU:HA    | 5        | 2.8           |
| (1,972)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HG    | 5        | 2.78          |
| (1,972)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HG    | 5        | 2.78          |
| (1,972)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HG    | 5        | 2.78          |
| (1,105)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HG    | 5        | 2.78          |
| (1,105)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HG    | 5        | 2.78          |
| (1,105)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HG    | 5        | 2.78          |
| (1,1754) | 1:A:118:PHE:HZ   | 1:B:116:ARG:HA   | 8        | 2.76          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD1   | 3        | 2.75          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD2   | 3        | 2.75          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD1   | 3        | 2.75          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD2   | 3        | 2.75          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG12 | 2        | 2.75          |
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG13 | 2        | 2.75          |
| (1,1189) | 1:B:97:VAL:HB    | 1:B:94:LEU:HA    | 8        | 2.75          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD1   | 3        | 2.75          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD2   | 3        | 2.75          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD1   | 3        | 2.75          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD2   | 3        | 2.75          |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG12 | 2        | 2.74          |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG13 | 2        | 2.74          |
| (1,618)  | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD1  | 6        | 2.74          |
| (1,618)  | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD2  | 6        | 2.74          |
| (1,618)  | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD1  | 6        | 2.74          |
| (1,618)  | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD2  | 6        | 2.74          |
| (1,618)  | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD1  | 6        | 2.74          |
| (1,618)  | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD2  | 6        | 2.74          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG21 | 6        | 2.74          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG22 | 6        | 2.74          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG23 | 6        | 2.74          |
| (1,322)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HA    | 8        | 2.74          |
| (1,1770) | 1:A:123:ARG:HD2  | 1:B:113:PHE:H    | 6        | 2.74          |
| (1,1770) | 1:A:123:ARG:HD3  | 1:B:113:PHE:H    | 6        | 2.74          |
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD1  | 6        | 2.74          |
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD2  | 6        | 2.74          |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD1  | 6        | 2.74          |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD2  | 6        | 2.74          |
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD1  | 6        | 2.74          |
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD2  | 6        | 2.74          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG21 | 6        | 2.74          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG22 | 6        | 2.74          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG23 | 6        | 2.74          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD1   | 8        | 2.74          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD2   | 8        | 2.74          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD1   | 8        | 2.74          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD2   | 8        | 2.74          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD1   | 8        | 2.73          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD2   | 8        | 2.73          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD1   | 8        | 2.73          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD2   | 8        | 2.73          |
| (1,502)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HB2  | 4        | 2.72          |
| (1,502)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HB2  | 4        | 2.72          |
| (1,502)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HB2  | 4        | 2.72          |
| (1,322)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HA    | 2        | 2.72          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1369) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HB2 | 4        | 2.72          |
| (1,1369) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HB2 | 4        | 2.72          |
| (1,1369) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HB2 | 4        | 2.72          |
| (1,1189) | 1:B:97:VAL:HB    | 1:B:94:LEU:HA   | 2        | 2.72          |
| (1,436)  | 1:A:107:ARG:HB2  | 1:A:109:ASP:H   | 4        | 2.71          |
| (1,1303) | 1:B:107:ARG:HB2  | 1:B:109:ASP:H   | 4        | 2.71          |
| (1,641)  | 1:A:124:ILE:HG21 | 1:A:148:PRO:HA  | 7        | 2.7           |
| (1,641)  | 1:A:124:ILE:HG22 | 1:A:148:PRO:HA  | 7        | 2.7           |
| (1,641)  | 1:A:124:ILE:HG23 | 1:A:148:PRO:HA  | 7        | 2.7           |
| (1,1508) | 1:B:124:ILE:HG21 | 1:B:148:PRO:HA  | 7        | 2.7           |
| (1,1508) | 1:B:124:ILE:HG22 | 1:B:148:PRO:HA  | 7        | 2.7           |
| (1,1508) | 1:B:124:ILE:HG23 | 1:B:148:PRO:HA  | 7        | 2.7           |
| (1,322)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HA   | 3        | 2.69          |
| (1,1189) | 1:B:97:VAL:HB    | 1:B:94:LEU:HA   | 3        | 2.69          |
| (1,322)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HA   | 4        | 2.68          |
| (1,1189) | 1:B:97:VAL:HB    | 1:B:94:LEU:HA   | 4        | 2.68          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD1  | 2        | 2.67          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD2  | 2        | 2.67          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD1  | 2        | 2.67          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD2  | 2        | 2.67          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD1 | 9        | 2.67          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD2 | 9        | 2.67          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD1 | 9        | 2.67          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD2 | 9        | 2.67          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD1 | 9        | 2.67          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD2 | 9        | 2.67          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD1  | 2        | 2.67          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD2  | 2        | 2.67          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD1  | 2        | 2.67          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD2  | 2        | 2.67          |
| (1,254)  | 1:A:89:LEU:HD11  | 1:A:91:VAL:HB   | 2        | 2.65          |
| (1,254)  | 1:A:89:LEU:HD12  | 1:A:91:VAL:HB   | 2        | 2.65          |
| (1,254)  | 1:A:89:LEU:HD13  | 1:A:91:VAL:HB   | 2        | 2.65          |
| (1,1121) | 1:B:89:LEU:HD11  | 1:B:91:VAL:HB   | 2        | 2.65          |
| (1,1121) | 1:B:89:LEU:HD12  | 1:B:91:VAL:HB   | 2        | 2.65          |
| (1,1121) | 1:B:89:LEU:HD13  | 1:B:91:VAL:HB   | 2        | 2.65          |
| (1,890)  | 1:B:70:LEU:HB2   | 1:B:74:ARG:H    | 3        | 2.64          |
| (1,986)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB3 | 6        | 2.63          |
| (1,434)  | 1:A:107:ARG:HD3  | 1:A:109:ASP:H   | 1        | 2.63          |
| (1,23)   | 1:A:70:LEU:HB2   | 1:A:74:ARG:H    | 3        | 2.63          |
| (1,1760) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H   | 6        | 2.63          |
| (1,1760) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H   | 6        | 2.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1301) | 1:B:107:ARG:HD3  | 1:B:109:ASP:H    | 1        | 2.63          |
| (1,119)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB3  | 6        | 2.63          |
| (1,643)  | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD1  | 6        | 2.62          |
| (1,643)  | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD2  | 6        | 2.62          |
| (1,436)  | 1:A:107:ARG:HB2  | 1:A:109:ASP:H    | 3        | 2.62          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD1   | 6        | 2.62          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD2   | 6        | 2.62          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD1   | 6        | 2.62          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD2   | 6        | 2.62          |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD1  | 6        | 2.62          |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD2  | 6        | 2.62          |
| (1,1303) | 1:B:107:ARG:HB2  | 1:B:109:ASP:H    | 3        | 2.62          |
| (1,520)  | 1:A:115:SER:HA   | 1:A:104:HIS:HE1  | 8        | 2.61          |
| (1,357)  | 1:A:100:VAL:HG11 | 1:A:80:ASP:HA    | 3        | 2.61          |
| (1,357)  | 1:A:100:VAL:HG12 | 1:A:80:ASP:HA    | 3        | 2.61          |
| (1,357)  | 1:A:100:VAL:HG13 | 1:A:80:ASP:HA    | 3        | 2.61          |
| (1,1387) | 1:B:115:SER:HA   | 1:B:104:HIS:HE1  | 8        | 2.61          |
| (1,1224) | 1:B:100:VAL:HG11 | 1:B:80:ASP:HA    | 3        | 2.61          |
| (1,1224) | 1:B:100:VAL:HG12 | 1:B:80:ASP:HA    | 3        | 2.61          |
| (1,1224) | 1:B:100:VAL:HG13 | 1:B:80:ASP:HA    | 3        | 2.61          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD1   | 6        | 2.61          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD2   | 6        | 2.61          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD1   | 6        | 2.61          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD2   | 6        | 2.61          |
| (1,322)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HA    | 7        | 2.6           |
| (1,322)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HA    | 9        | 2.6           |
| (1,1762) | 1:A:122:TYR:HB2  | 1:B:111:HIS:H    | 7        | 2.6           |
| (1,1762) | 1:A:122:TYR:HB3  | 1:B:111:HIS:H    | 7        | 2.6           |
| (1,1189) | 1:B:97:VAL:HB    | 1:B:94:LEU:HA    | 7        | 2.6           |
| (1,1189) | 1:B:97:VAL:HB    | 1:B:94:LEU:HA    | 9        | 2.6           |
| (1,850)  | 1:A:147:GLY:HA2  | 1:A:149:ARG:H    | 6        | 2.59          |
| (1,1717) | 1:B:147:GLY:HA2  | 1:B:149:ARG:H    | 6        | 2.59          |
| (1,850)  | 1:A:147:GLY:HA2  | 1:A:149:ARG:H    | 1        | 2.58          |
| (1,1717) | 1:B:147:GLY:HA2  | 1:B:149:ARG:H    | 1        | 2.58          |
| (1,986)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB3  | 9        | 2.57          |
| (1,619)  | 1:A:124:ILE:HA   | 1:A:122:TYR:HD1  | 6        | 2.57          |
| (1,619)  | 1:A:124:ILE:HA   | 1:A:122:TYR:HD2  | 6        | 2.57          |
| (1,1486) | 1:B:124:ILE:HA   | 1:B:122:TYR:HD1  | 6        | 2.57          |
| (1,1486) | 1:B:124:ILE:HA   | 1:B:122:TYR:HD2  | 6        | 2.57          |
| (1,119)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB3  | 9        | 2.57          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG21 | 1        | 2.53          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG22 | 1        | 2.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG23 | 1        | 2.53          |
| (1,421)  | 1:A:107:ARG:HD2  | 1:A:105:GLU:H    | 4        | 2.53          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG21 | 1        | 2.53          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG22 | 1        | 2.53          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG23 | 1        | 2.53          |
| (1,1288) | 1:B:107:ARG:HD2  | 1:B:105:GLU:H    | 4        | 2.53          |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG2  | 3        | 2.51          |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG3  | 3        | 2.51          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD1   | 7        | 2.51          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD2   | 7        | 2.51          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD1   | 7        | 2.51          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD2   | 7        | 2.51          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG2  | 3        | 2.51          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG3  | 3        | 2.51          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD1   | 7        | 2.51          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD2   | 7        | 2.51          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD1   | 7        | 2.51          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD2   | 7        | 2.51          |
| (1,850)  | 1:A:147:GLY:HA2  | 1:A:149:ARG:H    | 2        | 2.49          |
| (1,850)  | 1:A:147:GLY:HA2  | 1:A:149:ARG:H    | 5        | 2.49          |
| (1,1717) | 1:B:147:GLY:HA2  | 1:B:149:ARG:H    | 2        | 2.49          |
| (1,1717) | 1:B:147:GLY:HA2  | 1:B:149:ARG:H    | 5        | 2.49          |
| (1,889)  | 1:B:70:LEU:HB3   | 1:B:74:ARG:H     | 7        | 2.47          |
| (1,681)  | 1:A:128:VAL:H    | 1:A:150:LYS:HD2  | 8        | 2.47          |
| (1,681)  | 1:A:128:VAL:H    | 1:A:150:LYS:HD3  | 8        | 2.47          |
| (1,641)  | 1:A:124:ILE:HG21 | 1:A:148:PRO:HA   | 8        | 2.47          |
| (1,641)  | 1:A:124:ILE:HG22 | 1:A:148:PRO:HA   | 8        | 2.47          |
| (1,641)  | 1:A:124:ILE:HG23 | 1:A:148:PRO:HA   | 8        | 2.47          |
| (1,22)   | 1:A:70:LEU:HB3   | 1:A:74:ARG:H     | 7        | 2.47          |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD1  | 2        | 2.47          |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD2  | 2        | 2.47          |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD1  | 2        | 2.47          |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD2  | 2        | 2.47          |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD1  | 2        | 2.47          |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD2  | 2        | 2.47          |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD2  | 8        | 2.47          |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD3  | 8        | 2.47          |
| (1,1508) | 1:B:124:ILE:HG21 | 1:B:148:PRO:HA   | 8        | 2.47          |
| (1,1508) | 1:B:124:ILE:HG22 | 1:B:148:PRO:HA   | 8        | 2.47          |
| (1,1508) | 1:B:124:ILE:HG23 | 1:B:148:PRO:HA   | 8        | 2.47          |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD1  | 2        | 2.47          |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD2  | 2        | 2.47          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD1 | 2        | 2.47          |
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD2 | 2        | 2.47          |
| (1,1032) | 1:B:81:VAL:HG23  | 1:B:118:PHE:HD1 | 2        | 2.47          |
| (1,1032) | 1:B:81:VAL:HG23  | 1:B:118:PHE:HD2 | 2        | 2.47          |
| (1,850)  | 1:A:147:GLY:HA2  | 1:A:149:ARG:H   | 4        | 2.46          |
| (1,1717) | 1:B:147:GLY:HA2  | 1:B:149:ARG:H   | 4        | 2.46          |
| (1,434)  | 1:A:107:ARG:HD3  | 1:A:109:ASP:H   | 2        | 2.45          |
| (1,1301) | 1:B:107:ARG:HD3  | 1:B:109:ASP:H   | 2        | 2.45          |
| (1,1754) | 1:A:118:PHE:HZ   | 1:B:116:ARG:HA  | 2        | 2.44          |
| (1,850)  | 1:A:147:GLY:HA2  | 1:A:149:ARG:H   | 3        | 2.42          |
| (1,850)  | 1:A:147:GLY:HA2  | 1:A:149:ARG:H   | 9        | 2.42          |
| (1,1717) | 1:B:147:GLY:HA2  | 1:B:149:ARG:H   | 3        | 2.42          |
| (1,1717) | 1:B:147:GLY:HA2  | 1:B:149:ARG:H   | 9        | 2.42          |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD1 | 9        | 2.42          |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD2 | 9        | 2.42          |
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD1 | 9        | 2.42          |
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD2 | 9        | 2.42          |
| (1,1032) | 1:B:81:VAL:HG23  | 1:B:118:PHE:HD1 | 9        | 2.42          |
| (1,1032) | 1:B:81:VAL:HG23  | 1:B:118:PHE:HD2 | 9        | 2.42          |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD1 | 9        | 2.41          |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD2 | 9        | 2.41          |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD1 | 9        | 2.41          |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD2 | 9        | 2.41          |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD1 | 9        | 2.41          |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD2 | 9        | 2.41          |
| (1,641)  | 1:A:124:ILE:HG21 | 1:A:148:PRO:HA  | 9        | 2.4           |
| (1,641)  | 1:A:124:ILE:HG22 | 1:A:148:PRO:HA  | 9        | 2.4           |
| (1,641)  | 1:A:124:ILE:HG23 | 1:A:148:PRO:HA  | 9        | 2.4           |
| (1,1508) | 1:B:124:ILE:HG21 | 1:B:148:PRO:HA  | 9        | 2.4           |
| (1,1508) | 1:B:124:ILE:HG22 | 1:B:148:PRO:HA  | 9        | 2.4           |
| (1,1508) | 1:B:124:ILE:HG23 | 1:B:148:PRO:HA  | 9        | 2.4           |
| (1,641)  | 1:A:124:ILE:HG21 | 1:A:148:PRO:HA  | 5        | 2.39          |
| (1,641)  | 1:A:124:ILE:HG22 | 1:A:148:PRO:HA  | 5        | 2.39          |
| (1,641)  | 1:A:124:ILE:HG23 | 1:A:148:PRO:HA  | 5        | 2.39          |
| (1,1508) | 1:B:124:ILE:HG21 | 1:B:148:PRO:HA  | 5        | 2.39          |
| (1,1508) | 1:B:124:ILE:HG22 | 1:B:148:PRO:HA  | 5        | 2.39          |
| (1,1508) | 1:B:124:ILE:HG23 | 1:B:148:PRO:HA  | 5        | 2.39          |
| (1,890)  | 1:B:70:LEU:HB2   | 1:B:74:ARG:H    | 9        | 2.36          |
| (1,23)   | 1:A:70:LEU:HB2   | 1:A:74:ARG:H    | 9        | 2.36          |
| (1,523)  | 1:A:115:SER:HB3  | 1:A:106:GLU:H   | 2        | 2.32          |
| (1,455)  | 1:A:111:HIS:HA   | 1:A:109:ASP:HA  | 3        | 2.32          |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG2 | 9        | 2.32          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG3 | 9        | 2.32          |
| (1,1761) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H   | 9        | 2.32          |
| (1,1761) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H   | 9        | 2.32          |
| (1,1390) | 1:B:115:SER:HB3  | 1:B:106:GLU:H   | 2        | 2.32          |
| (1,1322) | 1:B:111:HIS:HA   | 1:B:109:ASP:HA  | 3        | 2.32          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG2 | 9        | 2.32          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG3 | 9        | 2.32          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB2 | 5        | 2.3           |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB3 | 5        | 2.3           |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB2 | 5        | 2.3           |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB3 | 5        | 2.3           |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB2 | 5        | 2.3           |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB3 | 5        | 2.3           |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD1  | 4        | 2.3           |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD2  | 4        | 2.3           |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD1  | 4        | 2.3           |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD2  | 4        | 2.3           |
| (1,185)  | 1:A:83:HIS:HB3   | 1:A:104:HIS:HB2 | 3        | 2.3           |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB2 | 5        | 2.3           |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB3 | 5        | 2.3           |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB2 | 5        | 2.3           |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB3 | 5        | 2.3           |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB2 | 5        | 2.3           |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB3 | 5        | 2.3           |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD1  | 4        | 2.3           |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD2  | 4        | 2.3           |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD1  | 4        | 2.3           |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD2  | 4        | 2.3           |
| (1,1052) | 1:B:83:HIS:HB3   | 1:B:104:HIS:HB2 | 3        | 2.3           |
| (1,501)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HE1 | 4        | 2.29          |
| (1,501)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HE1 | 4        | 2.29          |
| (1,501)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HE1 | 4        | 2.29          |
| (1,455)  | 1:A:111:HIS:HA   | 1:A:109:ASP:HA  | 8        | 2.29          |
| (1,1762) | 1:A:122:TYR:HB2  | 1:B:111:HIS:H   | 5        | 2.29          |
| (1,1762) | 1:A:122:TYR:HB3  | 1:B:111:HIS:H   | 5        | 2.29          |
| (1,1368) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HE1 | 4        | 2.29          |
| (1,1368) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HE1 | 4        | 2.29          |
| (1,1368) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HE1 | 4        | 2.29          |
| (1,1322) | 1:B:111:HIS:HA   | 1:B:109:ASP:HA  | 8        | 2.29          |
| (1,890)  | 1:B:70:LEU:HB2   | 1:B:74:ARG:H    | 7        | 2.28          |
| (1,641)  | 1:A:124:ILE:HG21 | 1:A:148:PRO:HA  | 3        | 2.28          |
| (1,641)  | 1:A:124:ILE:HG22 | 1:A:148:PRO:HA  | 3        | 2.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,641)  | 1:A:124:ILE:HG23 | 1:A:148:PRO:HA   | 3        | 2.28          |
| (1,434)  | 1:A:107:ARG:HD3  | 1:A:109:ASP:H    | 6        | 2.28          |
| (1,23)   | 1:A:70:LEU:HB2   | 1:A:74:ARG:H     | 7        | 2.28          |
| (1,1508) | 1:B:124:ILE:HG21 | 1:B:148:PRO:HA   | 3        | 2.28          |
| (1,1508) | 1:B:124:ILE:HG22 | 1:B:148:PRO:HA   | 3        | 2.28          |
| (1,1508) | 1:B:124:ILE:HG23 | 1:B:148:PRO:HA   | 3        | 2.28          |
| (1,1301) | 1:B:107:ARG:HD3  | 1:B:109:ASP:H    | 6        | 2.28          |
| (1,435)  | 1:A:107:ARG:HB3  | 1:A:109:ASP:H    | 1        | 2.27          |
| (1,1760) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H    | 1        | 2.27          |
| (1,1760) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H    | 1        | 2.27          |
| (1,1302) | 1:B:107:ARG:HB3  | 1:B:109:ASP:H    | 1        | 2.27          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB2  | 1        | 2.26          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB3  | 1        | 2.26          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB2  | 1        | 2.26          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB3  | 1        | 2.26          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB2  | 1        | 2.26          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB3  | 1        | 2.26          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB2  | 1        | 2.26          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB3  | 1        | 2.26          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB2  | 1        | 2.26          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB3  | 1        | 2.26          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB2  | 1        | 2.26          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB3  | 1        | 2.26          |
| (1,889)  | 1:B:70:LEU:HB3   | 1:B:74:ARG:H     | 9        | 2.25          |
| (1,22)   | 1:A:70:LEU:HB3   | 1:A:74:ARG:H     | 9        | 2.25          |
| (1,1322) | 1:B:111:HIS:HA   | 1:B:109:ASP:HA   | 9        | 2.25          |
| (1,455)  | 1:A:111:HIS:HA   | 1:A:109:ASP:HA   | 9        | 2.24          |
| (1,501)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HE1  | 6        | 2.23          |
| (1,501)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HE1  | 6        | 2.23          |
| (1,501)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HE1  | 6        | 2.23          |
| (1,455)  | 1:A:111:HIS:HA   | 1:A:109:ASP:HA   | 7        | 2.23          |
| (1,434)  | 1:A:107:ARG:HD3  | 1:A:109:ASP:H    | 5        | 2.23          |
| (1,1322) | 1:B:111:HIS:HA   | 1:B:109:ASP:HA   | 7        | 2.23          |
| (1,1301) | 1:B:107:ARG:HD3  | 1:B:109:ASP:H    | 5        | 2.23          |
| (1,525)  | 1:A:115:SER:HB3  | 1:A:107:ARG:H    | 3        | 2.22          |
| (1,452)  | 1:A:109:ASP:H    | 1:A:114:ILE:HG13 | 5        | 2.22          |
| (1,1392) | 1:B:115:SER:HB3  | 1:B:107:ARG:H    | 3        | 2.22          |
| (1,1368) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HE1  | 6        | 2.22          |
| (1,1368) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HE1  | 6        | 2.22          |
| (1,1368) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HE1  | 6        | 2.22          |
| (1,1319) | 1:B:109:ASP:H    | 1:B:114:ILE:HG13 | 5        | 2.22          |
| (1,455)  | 1:A:111:HIS:HA   | 1:A:109:ASP:HA   | 6        | 2.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1322) | 1:B:111:HIS:HA   | 1:B:109:ASP:HA   | 6        | 2.21          |
| (1,434)  | 1:A:107:ARG:HD3  | 1:A:109:ASP:H    | 9        | 2.2           |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD1  | 5        | 2.2           |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD2  | 5        | 2.2           |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD1  | 5        | 2.2           |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD2  | 5        | 2.2           |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD1  | 5        | 2.2           |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD2  | 5        | 2.2           |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD1  | 5        | 2.2           |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD2  | 5        | 2.2           |
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD1  | 5        | 2.2           |
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD2  | 5        | 2.2           |
| (1,1032) | 1:B:81:VAL:HG23  | 1:B:118:PHE:HD1  | 5        | 2.2           |
| (1,1032) | 1:B:81:VAL:HG23  | 1:B:118:PHE:HD2  | 5        | 2.2           |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB2  | 2        | 2.19          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB3  | 2        | 2.19          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB2  | 2        | 2.19          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB3  | 2        | 2.19          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB2  | 2        | 2.19          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB3  | 2        | 2.19          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB2  | 2        | 2.19          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB3  | 2        | 2.19          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB2  | 2        | 2.19          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB3  | 2        | 2.19          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB2  | 2        | 2.19          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB3  | 2        | 2.19          |
| (1,1301) | 1:B:107:ARG:HD3  | 1:B:109:ASP:H    | 9        | 2.19          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG21 | 8        | 2.18          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG22 | 8        | 2.18          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG23 | 8        | 2.18          |
| (1,511)  | 1:A:114:ILE:HG21 | 1:A:112:GLY:H    | 4        | 2.18          |
| (1,511)  | 1:A:114:ILE:HG22 | 1:A:112:GLY:H    | 4        | 2.18          |
| (1,511)  | 1:A:114:ILE:HG23 | 1:A:112:GLY:H    | 4        | 2.18          |
| (1,1762) | 1:A:122:TYR:HB2  | 1:B:111:HIS:H    | 9        | 2.18          |
| (1,1762) | 1:A:122:TYR:HB3  | 1:B:111:HIS:H    | 9        | 2.18          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG21 | 8        | 2.18          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG22 | 8        | 2.18          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG23 | 8        | 2.18          |
| (1,1378) | 1:B:114:ILE:HG21 | 1:B:112:GLY:H    | 4        | 2.18          |
| (1,1378) | 1:B:114:ILE:HG22 | 1:B:112:GLY:H    | 4        | 2.18          |
| (1,1378) | 1:B:114:ILE:HG23 | 1:B:112:GLY:H    | 4        | 2.18          |
| (1,525)  | 1:A:115:SER:HB3  | 1:A:107:ARG:H    | 2        | 2.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,452)  | 1:A:109:ASP:H    | 1:A:114:ILE:HG13 | 6        | 2.17          |
| (1,1392) | 1:B:115:SER:HB3  | 1:B:107:ARG:H    | 2        | 2.17          |
| (1,1319) | 1:B:109:ASP:H    | 1:B:114:ILE:HG13 | 6        | 2.17          |
| (1,618)  | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD1  | 5        | 2.16          |
| (1,618)  | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD2  | 5        | 2.16          |
| (1,618)  | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD1  | 5        | 2.16          |
| (1,618)  | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD2  | 5        | 2.16          |
| (1,618)  | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD1  | 5        | 2.16          |
| (1,618)  | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD2  | 5        | 2.16          |
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD1  | 5        | 2.16          |
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD2  | 5        | 2.16          |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD1  | 5        | 2.16          |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD2  | 5        | 2.16          |
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD1  | 5        | 2.16          |
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD2  | 5        | 2.16          |
| (1,982)  | 1:B:77:VAL:HG11  | 1:B:145:VAL:H    | 9        | 2.15          |
| (1,982)  | 1:B:77:VAL:HG12  | 1:B:145:VAL:H    | 9        | 2.15          |
| (1,982)  | 1:B:77:VAL:HG13  | 1:B:145:VAL:H    | 9        | 2.15          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB2  | 7        | 2.15          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB3  | 7        | 2.15          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB2  | 7        | 2.15          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB3  | 7        | 2.15          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB2  | 7        | 2.15          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB3  | 7        | 2.15          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB2  | 7        | 2.15          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB3  | 7        | 2.15          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB2  | 7        | 2.15          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB3  | 7        | 2.15          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB2  | 7        | 2.15          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB3  | 7        | 2.15          |
| (1,115)  | 1:A:77:VAL:HG11  | 1:A:145:VAL:H    | 9        | 2.15          |
| (1,115)  | 1:A:77:VAL:HG12  | 1:A:145:VAL:H    | 9        | 2.15          |
| (1,115)  | 1:A:77:VAL:HG13  | 1:A:145:VAL:H    | 9        | 2.15          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB2  | 6        | 2.14          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB3  | 6        | 2.14          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB2  | 6        | 2.14          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB3  | 6        | 2.14          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB2  | 6        | 2.14          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB3  | 6        | 2.14          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB2  | 9        | 2.14          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB3  | 9        | 2.14          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB2  | 9        | 2.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB3  | 9        | 2.14          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB2  | 9        | 2.14          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB3  | 9        | 2.14          |
| (1,1506) | 1:B:124:ILE:HD11 | 1:B:128:VAL:H    | 9        | 2.14          |
| (1,1506) | 1:B:124:ILE:HD12 | 1:B:128:VAL:H    | 9        | 2.14          |
| (1,1506) | 1:B:124:ILE:HD13 | 1:B:128:VAL:H    | 9        | 2.14          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB2  | 9        | 2.14          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB3  | 9        | 2.14          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB2  | 9        | 2.14          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB3  | 9        | 2.14          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB2  | 9        | 2.14          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB3  | 9        | 2.14          |
| (1,639)  | 1:A:124:ILE:HD11 | 1:A:128:VAL:H    | 9        | 2.13          |
| (1,639)  | 1:A:124:ILE:HD12 | 1:A:128:VAL:H    | 9        | 2.13          |
| (1,639)  | 1:A:124:ILE:HD13 | 1:A:128:VAL:H    | 9        | 2.13          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB2  | 6        | 2.13          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB3  | 6        | 2.13          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB2  | 6        | 2.13          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB3  | 6        | 2.13          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB2  | 6        | 2.13          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB3  | 6        | 2.13          |
| (1,520)  | 1:A:115:SER:HA   | 1:A:104:HIS:HE1  | 4        | 2.12          |
| (1,455)  | 1:A:111:HIS:HA   | 1:A:109:ASP:HA   | 2        | 2.12          |
| (1,1387) | 1:B:115:SER:HA   | 1:B:104:HIS:HE1  | 4        | 2.12          |
| (1,1322) | 1:B:111:HIS:HA   | 1:B:109:ASP:HA   | 2        | 2.12          |
| (1,890)  | 1:B:70:LEU:HB2   | 1:B:74:ARG:H     | 2        | 2.11          |
| (1,455)  | 1:A:111:HIS:HA   | 1:A:109:ASP:HA   | 4        | 2.11          |
| (1,23)   | 1:A:70:LEU:HB2   | 1:A:74:ARG:H     | 2        | 2.11          |
| (1,1322) | 1:B:111:HIS:HA   | 1:B:109:ASP:HA   | 4        | 2.11          |
| (1,681)  | 1:A:128:VAL:H    | 1:A:150:LYS:HD2  | 4        | 2.1           |
| (1,681)  | 1:A:128:VAL:H    | 1:A:150:LYS:HD3  | 4        | 2.1           |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD2  | 4        | 2.1           |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD3  | 4        | 2.1           |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD1  | 5        | 2.1           |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD2  | 5        | 2.1           |
| (1,643)  | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD1  | 5        | 2.09          |
| (1,643)  | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD2  | 5        | 2.09          |
| (1,641)  | 1:A:124:ILE:HG21 | 1:A:148:PRO:HA   | 6        | 2.09          |
| (1,641)  | 1:A:124:ILE:HG22 | 1:A:148:PRO:HA   | 6        | 2.09          |
| (1,641)  | 1:A:124:ILE:HG23 | 1:A:148:PRO:HA   | 6        | 2.09          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD11 | 1        | 2.09          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD12 | 1        | 2.09          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD13 | 1        | 2.09          |
| (1,520)  | 1:A:115:SER:HA   | 1:A:104:HIS:HE1  | 1        | 2.09          |
| (1,1508) | 1:B:124:ILE:HG21 | 1:B:148:PRO:HA   | 6        | 2.09          |
| (1,1508) | 1:B:124:ILE:HG22 | 1:B:148:PRO:HA   | 6        | 2.09          |
| (1,1508) | 1:B:124:ILE:HG23 | 1:B:148:PRO:HA   | 6        | 2.09          |
| (1,1387) | 1:B:115:SER:HA   | 1:B:104:HIS:HE1  | 1        | 2.09          |
| (1,619)  | 1:A:124:ILE:HA   | 1:A:122:TYR:HD1  | 5        | 2.08          |
| (1,619)  | 1:A:124:ILE:HA   | 1:A:122:TYR:HD2  | 5        | 2.08          |
| (1,520)  | 1:A:115:SER:HA   | 1:A:104:HIS:HE1  | 5        | 2.08          |
| (1,1486) | 1:B:124:ILE:HA   | 1:B:122:TYR:HD1  | 5        | 2.08          |
| (1,1486) | 1:B:124:ILE:HA   | 1:B:122:TYR:HD2  | 5        | 2.08          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD11 | 1        | 2.08          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD12 | 1        | 2.08          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD13 | 1        | 2.08          |
| (1,1387) | 1:B:115:SER:HA   | 1:B:104:HIS:HE1  | 5        | 2.08          |
| (1,890)  | 1:B:70:LEU:HB2   | 1:B:74:ARG:H     | 1        | 2.07          |
| (1,639)  | 1:A:124:ILE:HD11 | 1:A:128:VAL:H    | 5        | 2.07          |
| (1,639)  | 1:A:124:ILE:HD12 | 1:A:128:VAL:H    | 5        | 2.07          |
| (1,639)  | 1:A:124:ILE:HD13 | 1:A:128:VAL:H    | 5        | 2.07          |
| (1,23)   | 1:A:70:LEU:HB2   | 1:A:74:ARG:H     | 1        | 2.07          |
| (1,982)  | 1:B:77:VAL:HG11  | 1:B:145:VAL:H    | 6        | 2.06          |
| (1,982)  | 1:B:77:VAL:HG12  | 1:B:145:VAL:H    | 6        | 2.06          |
| (1,982)  | 1:B:77:VAL:HG13  | 1:B:145:VAL:H    | 6        | 2.06          |
| (1,639)  | 1:A:124:ILE:HD11 | 1:A:128:VAL:H    | 3        | 2.06          |
| (1,639)  | 1:A:124:ILE:HD12 | 1:A:128:VAL:H    | 3        | 2.06          |
| (1,639)  | 1:A:124:ILE:HD13 | 1:A:128:VAL:H    | 3        | 2.06          |
| (1,639)  | 1:A:124:ILE:HD11 | 1:A:128:VAL:H    | 7        | 2.06          |
| (1,639)  | 1:A:124:ILE:HD12 | 1:A:128:VAL:H    | 7        | 2.06          |
| (1,639)  | 1:A:124:ILE:HD13 | 1:A:128:VAL:H    | 7        | 2.06          |
| (1,525)  | 1:A:115:SER:HB3  | 1:A:107:ARG:H    | 8        | 2.06          |
| (1,452)  | 1:A:109:ASP:H    | 1:A:114:ILE:HG13 | 7        | 2.06          |
| (1,167)  | 1:A:81:VAL:H     | 1:A:141:GLY:HA2  | 3        | 2.06          |
| (1,1506) | 1:B:124:ILE:HD11 | 1:B:128:VAL:H    | 5        | 2.06          |
| (1,1506) | 1:B:124:ILE:HD12 | 1:B:128:VAL:H    | 5        | 2.06          |
| (1,1506) | 1:B:124:ILE:HD13 | 1:B:128:VAL:H    | 5        | 2.06          |
| (1,1392) | 1:B:115:SER:HB3  | 1:B:107:ARG:H    | 8        | 2.06          |
| (1,1319) | 1:B:109:ASP:H    | 1:B:114:ILE:HG13 | 7        | 2.06          |
| (1,115)  | 1:A:77:VAL:HG11  | 1:A:145:VAL:H    | 6        | 2.06          |
| (1,115)  | 1:A:77:VAL:HG12  | 1:A:145:VAL:H    | 6        | 2.06          |
| (1,115)  | 1:A:77:VAL:HG13  | 1:A:145:VAL:H    | 6        | 2.06          |
| (1,1034) | 1:B:81:VAL:H     | 1:B:141:GLY:HA2  | 3        | 2.06          |
| (1,1506) | 1:B:124:ILE:HD11 | 1:B:128:VAL:H    | 3        | 2.05          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1506) | 1:B:124:ILE:HD12 | 1:B:128:VAL:H    | 3        | 2.05          |
| (1,1506) | 1:B:124:ILE:HD13 | 1:B:128:VAL:H    | 3        | 2.05          |
| (1,1506) | 1:B:124:ILE:HD11 | 1:B:128:VAL:H    | 7        | 2.05          |
| (1,1506) | 1:B:124:ILE:HD12 | 1:B:128:VAL:H    | 7        | 2.05          |
| (1,1506) | 1:B:124:ILE:HD13 | 1:B:128:VAL:H    | 7        | 2.05          |
| (1,639)  | 1:A:124:ILE:HD11 | 1:A:128:VAL:H    | 8        | 2.04          |
| (1,639)  | 1:A:124:ILE:HD12 | 1:A:128:VAL:H    | 8        | 2.04          |
| (1,639)  | 1:A:124:ILE:HD13 | 1:A:128:VAL:H    | 8        | 2.04          |
| (1,439)  | 1:A:107:ARG:HD3  | 1:A:114:ILE:HG21 | 7        | 2.04          |
| (1,439)  | 1:A:107:ARG:HD3  | 1:A:114:ILE:HG22 | 7        | 2.04          |
| (1,439)  | 1:A:107:ARG:HD3  | 1:A:114:ILE:HG23 | 7        | 2.04          |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG2  | 7        | 2.04          |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG3  | 7        | 2.04          |
| (1,1506) | 1:B:124:ILE:HD11 | 1:B:128:VAL:H    | 1        | 2.04          |
| (1,1506) | 1:B:124:ILE:HD12 | 1:B:128:VAL:H    | 1        | 2.04          |
| (1,1506) | 1:B:124:ILE:HD13 | 1:B:128:VAL:H    | 1        | 2.04          |
| (1,1306) | 1:B:107:ARG:HD3  | 1:B:114:ILE:HG21 | 7        | 2.04          |
| (1,1306) | 1:B:107:ARG:HD3  | 1:B:114:ILE:HG22 | 7        | 2.04          |
| (1,1306) | 1:B:107:ARG:HD3  | 1:B:114:ILE:HG23 | 7        | 2.04          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG2  | 7        | 2.04          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG3  | 7        | 2.04          |
| (1,1506) | 1:B:124:ILE:HD11 | 1:B:128:VAL:H    | 8        | 2.03          |
| (1,1506) | 1:B:124:ILE:HD12 | 1:B:128:VAL:H    | 8        | 2.03          |
| (1,1506) | 1:B:124:ILE:HD13 | 1:B:128:VAL:H    | 8        | 2.03          |
| (1,1319) | 1:B:109:ASP:H    | 1:B:114:ILE:HG13 | 1        | 2.03          |
| (1,639)  | 1:A:124:ILE:HD11 | 1:A:128:VAL:H    | 1        | 2.02          |
| (1,639)  | 1:A:124:ILE:HD12 | 1:A:128:VAL:H    | 1        | 2.02          |
| (1,639)  | 1:A:124:ILE:HD13 | 1:A:128:VAL:H    | 1        | 2.02          |
| (1,639)  | 1:A:124:ILE:HD11 | 1:A:128:VAL:H    | 2        | 2.02          |
| (1,639)  | 1:A:124:ILE:HD12 | 1:A:128:VAL:H    | 2        | 2.02          |
| (1,639)  | 1:A:124:ILE:HD13 | 1:A:128:VAL:H    | 2        | 2.02          |
| (1,452)  | 1:A:109:ASP:H    | 1:A:114:ILE:HG13 | 1        | 2.02          |
| (1,1506) | 1:B:124:ILE:HD11 | 1:B:128:VAL:H    | 2        | 2.02          |
| (1,1506) | 1:B:124:ILE:HD12 | 1:B:128:VAL:H    | 2        | 2.02          |
| (1,1506) | 1:B:124:ILE:HD13 | 1:B:128:VAL:H    | 2        | 2.02          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG21 | 3        | 2.01          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG22 | 3        | 2.01          |
| (1,549)  | 1:A:118:PHE:HB2  | 1:A:100:VAL:HG23 | 3        | 2.01          |
| (1,501)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HE1  | 2        | 2.01          |
| (1,501)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HE1  | 2        | 2.01          |
| (1,501)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HE1  | 2        | 2.01          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG21 | 3        | 2.01          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG22 | 3        | 2.01          |
| (1,1416) | 1:B:118:PHE:HB2  | 1:B:100:VAL:HG23 | 3        | 2.01          |
| (1,1368) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HE1  | 2        | 2.01          |
| (1,1368) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HE1  | 2        | 2.01          |
| (1,1368) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HE1  | 2        | 2.01          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD1  | 1        | 2.0           |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD2  | 1        | 2.0           |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD1  | 1        | 2.0           |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD2  | 1        | 2.0           |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD1  | 1        | 2.0           |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD2  | 1        | 2.0           |
| (1,639)  | 1:A:124:ILE:HD11 | 1:A:128:VAL:H    | 6        | 1.99          |
| (1,639)  | 1:A:124:ILE:HD12 | 1:A:128:VAL:H    | 6        | 1.99          |
| (1,639)  | 1:A:124:ILE:HD13 | 1:A:128:VAL:H    | 6        | 1.99          |
| (1,1506) | 1:B:124:ILE:HD11 | 1:B:128:VAL:H    | 6        | 1.99          |
| (1,1506) | 1:B:124:ILE:HD12 | 1:B:128:VAL:H    | 6        | 1.99          |
| (1,1506) | 1:B:124:ILE:HD13 | 1:B:128:VAL:H    | 6        | 1.99          |
| (1,452)  | 1:A:109:ASP:H    | 1:A:114:ILE:HG13 | 9        | 1.96          |
| (1,321)  | 1:A:97:VAL:H     | 1:A:93:VAL:HB    | 5        | 1.96          |
| (1,22)   | 1:A:70:LEU:HB3   | 1:A:74:ARG:H     | 1        | 1.96          |
| (1,1319) | 1:B:109:ASP:H    | 1:B:114:ILE:HG13 | 9        | 1.96          |
| (1,889)  | 1:B:70:LEU:HB3   | 1:B:74:ARG:H     | 1        | 1.95          |
| (1,642)  | 1:A:125:PRO:HD3  | 1:A:122:TYR:HD1  | 6        | 1.95          |
| (1,642)  | 1:A:125:PRO:HD3  | 1:A:122:TYR:HD2  | 6        | 1.95          |
| (1,455)  | 1:A:111:HIS:HA   | 1:A:109:ASP:HA   | 1        | 1.95          |
| (1,1509) | 1:B:125:PRO:HD3  | 1:B:122:TYR:HD1  | 6        | 1.95          |
| (1,1509) | 1:B:125:PRO:HD3  | 1:B:122:TYR:HD2  | 6        | 1.95          |
| (1,1322) | 1:B:111:HIS:HA   | 1:B:109:ASP:HA   | 1        | 1.95          |
| (1,1188) | 1:B:97:VAL:H     | 1:B:93:VAL:HB    | 5        | 1.95          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD11 | 6        | 1.94          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD12 | 6        | 1.94          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD13 | 6        | 1.94          |
| (1,455)  | 1:A:111:HIS:HA   | 1:A:109:ASP:HA   | 5        | 1.94          |
| (1,421)  | 1:A:107:ARG:HD2  | 1:A:105:GLU:H    | 9        | 1.94          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD11 | 6        | 1.94          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD12 | 6        | 1.94          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD13 | 6        | 1.94          |
| (1,1322) | 1:B:111:HIS:HA   | 1:B:109:ASP:HA   | 5        | 1.94          |
| (1,1288) | 1:B:107:ARG:HD2  | 1:B:105:GLU:H    | 9        | 1.94          |
| (1,558)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HZ   | 9        | 1.92          |
| (1,188)  | 1:A:83:HIS:H     | 1:A:141:GLY:HA2  | 3        | 1.92          |
| (1,1055) | 1:B:83:HIS:H     | 1:B:141:GLY:HA2  | 3        | 1.92          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,890)  | 1:B:70:LEU:HB2   | 1:B:74:ARG:H    | 8        | 1.91          |
| (1,558)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HZ  | 4        | 1.91          |
| (1,23)   | 1:A:70:LEU:HB2   | 1:A:74:ARG:H    | 8        | 1.91          |
| (1,552)  | 1:A:118:PHE:HE1  | 1:A:103:LYS:H   | 7        | 1.9           |
| (1,552)  | 1:A:118:PHE:HE2  | 1:A:103:LYS:H   | 7        | 1.9           |
| (1,1425) | 1:B:118:PHE:HA   | 1:B:118:PHE:HZ  | 9        | 1.9           |
| (1,1419) | 1:B:118:PHE:HE1  | 1:B:103:LYS:H   | 7        | 1.9           |
| (1,1419) | 1:B:118:PHE:HE2  | 1:B:103:LYS:H   | 7        | 1.9           |
| (1,435)  | 1:A:107:ARG:HB3  | 1:A:109:ASP:H   | 9        | 1.89          |
| (1,1425) | 1:B:118:PHE:HA   | 1:B:118:PHE:HZ  | 4        | 1.89          |
| (1,1302) | 1:B:107:ARG:HB3  | 1:B:109:ASP:H   | 9        | 1.89          |
| (1,385)  | 1:A:102:GLY:HA2  | 1:A:84:PHE:HZ   | 7        | 1.88          |
| (1,641)  | 1:A:124:ILE:HG21 | 1:A:148:PRO:HA  | 1        | 1.87          |
| (1,641)  | 1:A:124:ILE:HG22 | 1:A:148:PRO:HA  | 1        | 1.87          |
| (1,641)  | 1:A:124:ILE:HG23 | 1:A:148:PRO:HA  | 1        | 1.87          |
| (1,1508) | 1:B:124:ILE:HG21 | 1:B:148:PRO:HA  | 1        | 1.87          |
| (1,1508) | 1:B:124:ILE:HG22 | 1:B:148:PRO:HA  | 1        | 1.87          |
| (1,1508) | 1:B:124:ILE:HG23 | 1:B:148:PRO:HA  | 1        | 1.87          |
| (1,555)  | 1:A:118:PHE:HB2  | 1:A:117:GLU:H   | 3        | 1.86          |
| (1,1422) | 1:B:118:PHE:HB2  | 1:B:117:GLU:H   | 3        | 1.86          |
| (1,385)  | 1:A:102:GLY:HA2  | 1:A:84:PHE:HZ   | 2        | 1.85          |
| (1,1252) | 1:B:102:GLY:HA2  | 1:B:84:PHE:HZ   | 2        | 1.85          |
| (1,1252) | 1:B:102:GLY:HA2  | 1:B:84:PHE:HZ   | 7        | 1.85          |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE1  | 2        | 1.84          |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE2  | 2        | 1.84          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE1  | 2        | 1.84          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE2  | 2        | 1.84          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE1  | 2        | 1.84          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE2  | 2        | 1.84          |
| (1,481)  | 1:A:113:PHE:HA   | 1:A:107:ARG:HB2 | 5        | 1.84          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE1  | 2        | 1.84          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE2  | 2        | 1.84          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE1  | 2        | 1.84          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE2  | 2        | 1.84          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE1  | 2        | 1.84          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE2  | 2        | 1.84          |
| (1,1348) | 1:B:113:PHE:HA   | 1:B:107:ARG:HB2 | 5        | 1.84          |
| (1,906)  | 1:B:74:ARG:HG2   | 1:B:73:ASP:H    | 7        | 1.82          |
| (1,906)  | 1:B:74:ARG:HG3   | 1:B:73:ASP:H    | 7        | 1.82          |
| (1,558)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HZ  | 5        | 1.82          |
| (1,39)   | 1:A:74:ARG:HG2   | 1:A:73:ASP:H    | 7        | 1.82          |
| (1,39)   | 1:A:74:ARG:HG3   | 1:A:73:ASP:H    | 7        | 1.82          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,385)  | 1:A:102:GLY:HA2  | 1:A:84:PHE:HZ    | 9        | 1.82          |
| (1,1425) | 1:B:118:PHE:HA   | 1:B:118:PHE:HZ   | 5        | 1.82          |
| (1,1252) | 1:B:102:GLY:HA2  | 1:B:84:PHE:HZ    | 9        | 1.82          |
| (1,502)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HB2  | 1        | 1.81          |
| (1,502)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HB2  | 1        | 1.81          |
| (1,502)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HB2  | 1        | 1.81          |
| (1,1754) | 1:A:118:PHE:HZ   | 1:B:116:ARG:HA   | 3        | 1.81          |
| (1,1369) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HB2  | 1        | 1.81          |
| (1,1369) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HB2  | 1        | 1.81          |
| (1,1369) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HB2  | 1        | 1.81          |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG12 | 4        | 1.8           |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG13 | 4        | 1.8           |
| (1,421)  | 1:A:107:ARG:HD2  | 1:A:105:GLU:H    | 1        | 1.8           |
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG12 | 4        | 1.8           |
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG13 | 4        | 1.8           |
| (1,1288) | 1:B:107:ARG:HD2  | 1:B:105:GLU:H    | 1        | 1.8           |
| (1,452)  | 1:A:109:ASP:H    | 1:A:114:ILE:HG13 | 2        | 1.78          |
| (1,1767) | 1:A:122:TYR:HB2  | 1:B:112:GLY:HA3  | 9        | 1.78          |
| (1,1767) | 1:A:122:TYR:HB3  | 1:B:112:GLY:HA3  | 9        | 1.78          |
| (1,1319) | 1:B:109:ASP:H    | 1:B:114:ILE:HG13 | 2        | 1.78          |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG12 | 7        | 1.77          |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG13 | 7        | 1.77          |
| (1,525)  | 1:A:115:SER:HB3  | 1:A:107:ARG:H    | 9        | 1.77          |
| (1,435)  | 1:A:107:ARG:HB3  | 1:A:109:ASP:H    | 6        | 1.77          |
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG12 | 7        | 1.77          |
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG13 | 7        | 1.77          |
| (1,1392) | 1:B:115:SER:HB3  | 1:B:107:ARG:H    | 9        | 1.77          |
| (1,1302) | 1:B:107:ARG:HB3  | 1:B:109:ASP:H    | 6        | 1.77          |
| (1,1252) | 1:B:102:GLY:HA2  | 1:B:84:PHE:HZ    | 3        | 1.77          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB2  | 3        | 1.76          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB3  | 3        | 1.76          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB2  | 3        | 1.76          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB3  | 3        | 1.76          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB2  | 3        | 1.76          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB3  | 3        | 1.76          |
| (1,435)  | 1:A:107:ARG:HB3  | 1:A:109:ASP:H    | 2        | 1.76          |
| (1,385)  | 1:A:102:GLY:HA2  | 1:A:84:PHE:HZ    | 3        | 1.76          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB2  | 3        | 1.76          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB3  | 3        | 1.76          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB2  | 3        | 1.76          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB3  | 3        | 1.76          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB2  | 3        | 1.76          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB3  | 3        | 1.76          |
| (1,1302) | 1:B:107:ARG:HB3  | 1:B:109:ASP:H    | 2        | 1.76          |
| (1,889)  | 1:B:70:LEU:HB3   | 1:B:74:ARG:H     | 4        | 1.75          |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG2  | 2        | 1.75          |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG3  | 2        | 1.75          |
| (1,22)   | 1:A:70:LEU:HB3   | 1:A:74:ARG:H     | 4        | 1.75          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG12 | 7        | 1.75          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG13 | 7        | 1.75          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG2  | 2        | 1.75          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG3  | 2        | 1.75          |
| (1,889)  | 1:B:70:LEU:HB3   | 1:B:74:ARG:H     | 5        | 1.74          |
| (1,525)  | 1:A:115:SER:HB3  | 1:A:107:ARG:H    | 6        | 1.74          |
| (1,22)   | 1:A:70:LEU:HB3   | 1:A:74:ARG:H     | 5        | 1.74          |
| (1,1392) | 1:B:115:SER:HB3  | 1:B:107:ARG:H    | 6        | 1.74          |
| (1,1288) | 1:B:107:ARG:HD2  | 1:B:105:GLU:H    | 2        | 1.74          |
| (1,435)  | 1:A:107:ARG:HB3  | 1:A:109:ASP:H    | 5        | 1.73          |
| (1,421)  | 1:A:107:ARG:HD2  | 1:A:105:GLU:H    | 2        | 1.73          |
| (1,1302) | 1:B:107:ARG:HB3  | 1:B:109:ASP:H    | 5        | 1.73          |
| (1,1264) | 1:B:103:LYS:HG2  | 1:B:116:ARG:H    | 9        | 1.73          |
| (1,1264) | 1:B:103:LYS:HG3  | 1:B:116:ARG:H    | 9        | 1.73          |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB2   | 8        | 1.72          |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB3   | 8        | 1.72          |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB2   | 8        | 1.72          |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB3   | 8        | 1.72          |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB2   | 8        | 1.72          |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB3   | 8        | 1.72          |
| (1,555)  | 1:A:118:PHE:HB2  | 1:A:117:GLU:H    | 5        | 1.72          |
| (1,397)  | 1:A:103:LYS:HG2  | 1:A:116:ARG:H    | 9        | 1.72          |
| (1,397)  | 1:A:103:LYS:HG3  | 1:A:116:ARG:H    | 9        | 1.72          |
| (1,1422) | 1:B:118:PHE:HB2  | 1:B:117:GLU:H    | 5        | 1.72          |
| (1,985)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB2  | 4        | 1.71          |
| (1,618)  | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD1  | 9        | 1.71          |
| (1,618)  | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD2  | 9        | 1.71          |
| (1,618)  | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD1  | 9        | 1.71          |
| (1,618)  | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD2  | 9        | 1.71          |
| (1,618)  | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD1  | 9        | 1.71          |
| (1,618)  | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD2  | 9        | 1.71          |
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD1  | 9        | 1.71          |
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD2  | 9        | 1.71          |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD1  | 9        | 1.71          |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD2  | 9        | 1.71          |
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD1  | 9        | 1.71          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD2 | 9        | 1.71          |
| (1,118)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB2 | 4        | 1.71          |
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB2  | 8        | 1.71          |
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB3  | 8        | 1.71          |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB2  | 8        | 1.71          |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB3  | 8        | 1.71          |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB2  | 8        | 1.71          |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB3  | 8        | 1.71          |
| (1,483)  | 1:A:113:PHE:HE1  | 1:A:107:ARG:HA  | 8        | 1.7           |
| (1,483)  | 1:A:113:PHE:HE2  | 1:A:107:ARG:HA  | 8        | 1.7           |
| (1,1350) | 1:B:113:PHE:HE1  | 1:B:107:ARG:HA  | 8        | 1.7           |
| (1,1350) | 1:B:113:PHE:HE2  | 1:B:107:ARG:HA  | 8        | 1.7           |
| (1,525)  | 1:A:115:SER:HB3  | 1:A:107:ARG:H   | 4        | 1.69          |
| (1,1761) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H   | 3        | 1.69          |
| (1,1761) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H   | 3        | 1.69          |
| (1,1760) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H   | 9        | 1.69          |
| (1,1760) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H   | 9        | 1.69          |
| (1,1392) | 1:B:115:SER:HB3  | 1:B:107:ARG:H   | 4        | 1.69          |
| (1,985)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB2 | 8        | 1.68          |
| (1,744)  | 1:A:135:SER:HB3  | 1:A:146:ASP:H   | 8        | 1.68          |
| (1,368)  | 1:A:101:HIS:HB2  | 1:A:92:LYS:HB2  | 2        | 1.68          |
| (1,368)  | 1:A:101:HIS:HB2  | 1:A:92:LYS:HB3  | 2        | 1.68          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB2  | 2        | 1.68          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB3  | 2        | 1.68          |
| (1,1611) | 1:B:135:SER:HB3  | 1:B:146:ASP:H   | 8        | 1.68          |
| (1,1235) | 1:B:101:HIS:HB2  | 1:B:92:LYS:HB2  | 2        | 1.68          |
| (1,1235) | 1:B:101:HIS:HB2  | 1:B:92:LYS:HB3  | 2        | 1.68          |
| (1,118)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB2 | 8        | 1.68          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB2  | 2        | 1.68          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB3  | 2        | 1.68          |
| (1,890)  | 1:B:70:LEU:HB2   | 1:B:74:ARG:H    | 4        | 1.67          |
| (1,886)  | 1:B:70:LEU:HD11  | 1:B:70:LEU:H    | 2        | 1.67          |
| (1,886)  | 1:B:70:LEU:HD12  | 1:B:70:LEU:H    | 2        | 1.67          |
| (1,886)  | 1:B:70:LEU:HD13  | 1:B:70:LEU:H    | 2        | 1.67          |
| (1,886)  | 1:B:70:LEU:HD21  | 1:B:70:LEU:H    | 2        | 1.67          |
| (1,886)  | 1:B:70:LEU:HD22  | 1:B:70:LEU:H    | 2        | 1.67          |
| (1,886)  | 1:B:70:LEU:HD23  | 1:B:70:LEU:H    | 2        | 1.67          |
| (1,885)  | 1:B:70:LEU:HD11  | 1:B:70:LEU:H    | 2        | 1.67          |
| (1,885)  | 1:B:70:LEU:HD12  | 1:B:70:LEU:H    | 2        | 1.67          |
| (1,885)  | 1:B:70:LEU:HD13  | 1:B:70:LEU:H    | 2        | 1.67          |
| (1,885)  | 1:B:70:LEU:HD21  | 1:B:70:LEU:H    | 2        | 1.67          |
| (1,885)  | 1:B:70:LEU:HD22  | 1:B:70:LEU:H    | 2        | 1.67          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,885)  | 1:B:70:LEU:HD23  | 1:B:70:LEU:H     | 2        | 1.67          |
| (1,452)  | 1:A:109:ASP:H    | 1:A:114:ILE:HG13 | 3        | 1.67          |
| (1,435)  | 1:A:107:ARG:HB3  | 1:A:109:ASP:H    | 7        | 1.67          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB2   | 8        | 1.67          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB3   | 8        | 1.67          |
| (1,23)   | 1:A:70:LEU:HB2   | 1:A:74:ARG:H     | 4        | 1.67          |
| (1,19)   | 1:A:70:LEU:HD11  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,19)   | 1:A:70:LEU:HD12  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,19)   | 1:A:70:LEU:HD13  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,19)   | 1:A:70:LEU:HD21  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,19)   | 1:A:70:LEU:HD22  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,19)   | 1:A:70:LEU:HD23  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,18)   | 1:A:70:LEU:HD11  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,18)   | 1:A:70:LEU:HD12  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,18)   | 1:A:70:LEU:HD13  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,18)   | 1:A:70:LEU:HD21  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,18)   | 1:A:70:LEU:HD22  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,18)   | 1:A:70:LEU:HD23  | 1:A:70:LEU:H     | 2        | 1.67          |
| (1,1319) | 1:B:109:ASP:H    | 1:B:114:ILE:HG13 | 3        | 1.67          |
| (1,1302) | 1:B:107:ARG:HB3  | 1:B:109:ASP:H    | 7        | 1.67          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB2   | 8        | 1.67          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB3   | 8        | 1.67          |
| (1,501)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HE1  | 9        | 1.66          |
| (1,501)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HE1  | 9        | 1.66          |
| (1,501)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HE1  | 9        | 1.66          |
| (1,1368) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HE1  | 9        | 1.66          |
| (1,1368) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HE1  | 9        | 1.66          |
| (1,1368) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HE1  | 9        | 1.66          |
| (1,976)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:H     | 1        | 1.65          |
| (1,976)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:H     | 1        | 1.65          |
| (1,976)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:H     | 1        | 1.65          |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB2   | 7        | 1.65          |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB3   | 7        | 1.65          |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB2   | 7        | 1.65          |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB3   | 7        | 1.65          |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB2   | 7        | 1.65          |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB3   | 7        | 1.65          |
| (1,435)  | 1:A:107:ARG:HB3  | 1:A:109:ASP:H    | 8        | 1.65          |
| (1,1302) | 1:B:107:ARG:HB3  | 1:B:109:ASP:H    | 8        | 1.65          |
| (1,109)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:H     | 1        | 1.65          |
| (1,109)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:H     | 1        | 1.65          |
| (1,109)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:H     | 1        | 1.65          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB2  | 7        | 1.65          |
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB3  | 7        | 1.65          |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB2  | 7        | 1.65          |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB3  | 7        | 1.65          |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB2  | 7        | 1.65          |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB3  | 7        | 1.65          |
| (1,880)  | 1:B:68:MET:HE1   | 1:B:122:TYR:HE1 | 8        | 1.64          |
| (1,880)  | 1:B:68:MET:HE1   | 1:B:122:TYR:HE2 | 8        | 1.64          |
| (1,880)  | 1:B:68:MET:HE2   | 1:B:122:TYR:HE1 | 8        | 1.64          |
| (1,880)  | 1:B:68:MET:HE2   | 1:B:122:TYR:HE2 | 8        | 1.64          |
| (1,880)  | 1:B:68:MET:HE3   | 1:B:122:TYR:HE1 | 8        | 1.64          |
| (1,880)  | 1:B:68:MET:HE3   | 1:B:122:TYR:HE2 | 8        | 1.64          |
| (1,813)  | 1:A:145:VAL:HA   | 1:A:135:SER:H   | 7        | 1.64          |
| (1,203)  | 1:A:84:PHE:HE1   | 1:A:116:ARG:H   | 5        | 1.64          |
| (1,203)  | 1:A:84:PHE:HE2   | 1:A:116:ARG:H   | 5        | 1.64          |
| (1,1680) | 1:B:145:VAL:HA   | 1:B:135:SER:H   | 7        | 1.64          |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE1 | 8        | 1.64          |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE2 | 8        | 1.64          |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE1 | 8        | 1.64          |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE2 | 8        | 1.64          |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE1 | 8        | 1.64          |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE2 | 8        | 1.64          |
| (1,813)  | 1:A:145:VAL:HA   | 1:A:135:SER:H   | 9        | 1.63          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB2  | 6        | 1.63          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB3  | 6        | 1.63          |
| (1,194)  | 1:A:84:PHE:HD1   | 1:A:83:HIS:H    | 3        | 1.63          |
| (1,194)  | 1:A:84:PHE:HD2   | 1:A:83:HIS:H    | 3        | 1.63          |
| (1,1680) | 1:B:145:VAL:HA   | 1:B:135:SER:H   | 9        | 1.63          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB2  | 6        | 1.63          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB3  | 6        | 1.63          |
| (1,1070) | 1:B:84:PHE:HE1   | 1:B:116:ARG:H   | 5        | 1.63          |
| (1,1070) | 1:B:84:PHE:HE2   | 1:B:116:ARG:H   | 5        | 1.63          |
| (1,1061) | 1:B:84:PHE:HD1   | 1:B:83:HIS:H    | 3        | 1.63          |
| (1,1061) | 1:B:84:PHE:HD2   | 1:B:83:HIS:H    | 3        | 1.63          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG2  | 6        | 1.62          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG3  | 6        | 1.62          |
| (1,502)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HB2 | 2        | 1.62          |
| (1,502)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HB2 | 2        | 1.62          |
| (1,502)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HB2 | 2        | 1.62          |
| (1,483)  | 1:A:113:PHE:HE1  | 1:A:107:ARG:HA  | 2        | 1.62          |
| (1,483)  | 1:A:113:PHE:HE2  | 1:A:107:ARG:HA  | 2        | 1.62          |
| (1,444)  | 1:A:108:GLN:HA   | 1:A:113:PHE:HE1 | 2        | 1.62          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,444)  | 1:A:108:GLN:HA   | 1:A:113:PHE:HE2  | 2        | 1.62          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB2   | 5        | 1.62          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB3   | 5        | 1.62          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG2   | 6        | 1.62          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG3   | 6        | 1.62          |
| (1,1369) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HB2  | 2        | 1.62          |
| (1,1369) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HB2  | 2        | 1.62          |
| (1,1369) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HB2  | 2        | 1.62          |
| (1,1350) | 1:B:113:PHE:HE1  | 1:B:107:ARG:HA   | 2        | 1.62          |
| (1,1350) | 1:B:113:PHE:HE2  | 1:B:107:ARG:HA   | 2        | 1.62          |
| (1,1311) | 1:B:108:GLN:HA   | 1:B:113:PHE:HE1  | 2        | 1.62          |
| (1,1311) | 1:B:108:GLN:HA   | 1:B:113:PHE:HE2  | 2        | 1.62          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB2   | 5        | 1.62          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB3   | 5        | 1.62          |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB2   | 1        | 1.61          |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB3   | 1        | 1.61          |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB2   | 1        | 1.61          |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB3   | 1        | 1.61          |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB2   | 1        | 1.61          |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB3   | 1        | 1.61          |
| (1,744)  | 1:A:135:SER:HB3  | 1:A:146:ASP:H    | 7        | 1.61          |
| (1,1745) | 1:A:114:ILE:H    | 1:B:121:LYS:H    | 2        | 1.61          |
| (1,170)  | 1:A:83:HIS:H     | 1:A:81:VAL:HB    | 2        | 1.61          |
| (1,1611) | 1:B:135:SER:HB3  | 1:B:146:ASP:H    | 7        | 1.61          |
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB2   | 1        | 1.61          |
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB3   | 1        | 1.61          |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB2   | 1        | 1.61          |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB3   | 1        | 1.61          |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB2   | 1        | 1.61          |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB3   | 1        | 1.61          |
| (1,1037) | 1:B:83:HIS:H     | 1:B:81:VAL:HB    | 2        | 1.61          |
| (1,976)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:H     | 7        | 1.6           |
| (1,976)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:H     | 7        | 1.6           |
| (1,976)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:H     | 7        | 1.6           |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB2   | 4        | 1.6           |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB3   | 4        | 1.6           |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB2   | 7        | 1.6           |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB3   | 7        | 1.6           |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG12 | 8        | 1.6           |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG13 | 8        | 1.6           |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB2   | 4        | 1.6           |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB3   | 4        | 1.6           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB2  | 7        | 1.6           |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB3  | 7        | 1.6           |
| (1,109)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:H    | 7        | 1.6           |
| (1,109)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:H    | 7        | 1.6           |
| (1,109)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:H    | 7        | 1.6           |
| (1,985)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB2 | 7        | 1.59          |
| (1,595)  | 1:A:122:TYR:HD1  | 1:A:122:TYR:H   | 7        | 1.59          |
| (1,595)  | 1:A:122:TYR:HD2  | 1:A:122:TYR:H   | 7        | 1.59          |
| (1,501)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HE1 | 1        | 1.59          |
| (1,501)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HE1 | 1        | 1.59          |
| (1,501)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HE1 | 1        | 1.59          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB2  | 9        | 1.59          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB3  | 9        | 1.59          |
| (1,1462) | 1:B:122:TYR:HD1  | 1:B:122:TYR:H   | 7        | 1.59          |
| (1,1462) | 1:B:122:TYR:HD2  | 1:B:122:TYR:H   | 7        | 1.59          |
| (1,118)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB2 | 7        | 1.59          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB2  | 9        | 1.59          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB3  | 9        | 1.59          |
| (1,985)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB2 | 3        | 1.58          |
| (1,555)  | 1:A:118:PHE:HB2  | 1:A:117:GLU:H   | 4        | 1.58          |
| (1,483)  | 1:A:113:PHE:HE1  | 1:A:107:ARG:HA  | 6        | 1.58          |
| (1,483)  | 1:A:113:PHE:HE2  | 1:A:107:ARG:HA  | 6        | 1.58          |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG2 | 5        | 1.58          |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG3 | 5        | 1.58          |
| (1,167)  | 1:A:81:VAL:H     | 1:A:141:GLY:HA2 | 5        | 1.58          |
| (1,1368) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HE1 | 1        | 1.58          |
| (1,1368) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HE1 | 1        | 1.58          |
| (1,1368) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HE1 | 1        | 1.58          |
| (1,1350) | 1:B:113:PHE:HE1  | 1:B:107:ARG:HA  | 6        | 1.58          |
| (1,1350) | 1:B:113:PHE:HE2  | 1:B:107:ARG:HA  | 6        | 1.58          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG2 | 5        | 1.58          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG3 | 5        | 1.58          |
| (1,118)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB2 | 3        | 1.58          |
| (1,1034) | 1:B:81:VAL:H     | 1:B:141:GLY:HA2 | 5        | 1.58          |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB2  | 3        | 1.57          |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB3  | 3        | 1.57          |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB2  | 3        | 1.57          |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB3  | 3        | 1.57          |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB2  | 3        | 1.57          |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB3  | 3        | 1.57          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD11 | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD12 | 5        | 1.57          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,879)  | 1:B:68:MET:HE1  | 1:B:70:LEU:HD13  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE1  | 1:B:70:LEU:HD21  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE1  | 1:B:70:LEU:HD22  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE1  | 1:B:70:LEU:HD23  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD11  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD12  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD13  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD21  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD22  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE2  | 1:B:70:LEU:HD23  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD11  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD12  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD13  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD21  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD22  | 5        | 1.57          |
| (1,879)  | 1:B:68:MET:HE3  | 1:B:70:LEU:HD23  | 5        | 1.57          |
| (1,1422) | 1:B:118:PHE:HB2 | 1:B:117:GLU:H    | 4        | 1.57          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD11  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD12  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD13  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD21  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD22  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD23  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD11  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD12  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD13  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD21  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD22  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD23  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD11  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD12  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD13  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD21  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD22  | 5        | 1.57          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD23  | 5        | 1.57          |
| (1,104)  | 1:A:77:VAL:HG21 | 1:A:79:LEU:HB2   | 3        | 1.57          |
| (1,104)  | 1:A:77:VAL:HG21 | 1:A:79:LEU:HB3   | 3        | 1.57          |
| (1,104)  | 1:A:77:VAL:HG22 | 1:A:79:LEU:HB2   | 3        | 1.57          |
| (1,104)  | 1:A:77:VAL:HG22 | 1:A:79:LEU:HB3   | 3        | 1.57          |
| (1,104)  | 1:A:77:VAL:HG23 | 1:A:79:LEU:HB2   | 3        | 1.57          |
| (1,104)  | 1:A:77:VAL:HG23 | 1:A:79:LEU:HB3   | 3        | 1.57          |
| (1,702)  | 1:A:132:THR:HB  | 1:A:133:ILE:HG12 | 6        | 1.56          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,702)  | 1:A:132:THR:HB  | 1:A:133:ILE:HG13 | 6        | 1.56          |
| (1,525)  | 1:A:115:SER:HB3 | 1:A:107:ARG:H    | 1        | 1.56          |
| (1,1569) | 1:B:132:THR:HB  | 1:B:133:ILE:HG12 | 6        | 1.56          |
| (1,1569) | 1:B:132:THR:HB  | 1:B:133:ILE:HG13 | 6        | 1.56          |
| (1,1392) | 1:B:115:SER:HB3 | 1:B:107:ARG:H    | 1        | 1.56          |
| (1,702)  | 1:A:132:THR:HB  | 1:A:133:ILE:HG12 | 1        | 1.55          |
| (1,702)  | 1:A:132:THR:HB  | 1:A:133:ILE:HG13 | 1        | 1.55          |
| (1,319)  | 1:A:96:ASP:H    | 1:A:123:ARG:HG2  | 8        | 1.55          |
| (1,319)  | 1:A:96:ASP:H    | 1:A:123:ARG:HG3  | 8        | 1.55          |
| (1,188)  | 1:A:83:HIS:H    | 1:A:141:GLY:HA2  | 8        | 1.55          |
| (1,1569) | 1:B:132:THR:HB  | 1:B:133:ILE:HG12 | 1        | 1.55          |
| (1,1569) | 1:B:132:THR:HB  | 1:B:133:ILE:HG13 | 1        | 1.55          |
| (1,1186) | 1:B:96:ASP:H    | 1:B:123:ARG:HG2  | 8        | 1.55          |
| (1,1186) | 1:B:96:ASP:H    | 1:B:123:ARG:HG3  | 8        | 1.55          |
| (1,1055) | 1:B:83:HIS:H    | 1:B:141:GLY:HA2  | 8        | 1.55          |
| (1,744)  | 1:A:135:SER:HB3 | 1:A:146:ASP:H    | 9        | 1.54          |
| (1,555)  | 1:A:118:PHE:HB2 | 1:A:117:GLU:H    | 6        | 1.54          |
| (1,434)  | 1:A:107:ARG:HD3 | 1:A:109:ASP:H    | 8        | 1.54          |
| (1,319)  | 1:A:96:ASP:H    | 1:A:123:ARG:HG2  | 4        | 1.54          |
| (1,319)  | 1:A:96:ASP:H    | 1:A:123:ARG:HG3  | 4        | 1.54          |
| (1,1611) | 1:B:135:SER:HB3 | 1:B:146:ASP:H    | 9        | 1.54          |
| (1,1422) | 1:B:118:PHE:HB2 | 1:B:117:GLU:H    | 6        | 1.54          |
| (1,1301) | 1:B:107:ARG:HD3 | 1:B:109:ASP:H    | 8        | 1.54          |
| (1,1186) | 1:B:96:ASP:H    | 1:B:123:ARG:HG2  | 4        | 1.54          |
| (1,1186) | 1:B:96:ASP:H    | 1:B:123:ARG:HG3  | 4        | 1.54          |
| (1,986)  | 1:B:77:VAL:HB   | 1:B:146:ASP:HB3  | 1        | 1.53          |
| (1,890)  | 1:B:70:LEU:HB2  | 1:B:74:ARG:H     | 5        | 1.53          |
| (1,23)   | 1:A:70:LEU:HB2  | 1:A:74:ARG:H     | 5        | 1.53          |
| (1,1767) | 1:A:122:TYR:HB2 | 1:B:112:GLY:HA3  | 7        | 1.53          |
| (1,1767) | 1:A:122:TYR:HB3 | 1:B:112:GLY:HA3  | 7        | 1.53          |
| (1,165)  | 1:A:81:VAL:HG21 | 1:A:118:PHE:HD1  | 3        | 1.53          |
| (1,165)  | 1:A:81:VAL:HG21 | 1:A:118:PHE:HD2  | 3        | 1.53          |
| (1,165)  | 1:A:81:VAL:HG22 | 1:A:118:PHE:HD1  | 3        | 1.53          |
| (1,165)  | 1:A:81:VAL:HG22 | 1:A:118:PHE:HD2  | 3        | 1.53          |
| (1,165)  | 1:A:81:VAL:HG23 | 1:A:118:PHE:HD1  | 3        | 1.53          |
| (1,165)  | 1:A:81:VAL:HG23 | 1:A:118:PHE:HD2  | 3        | 1.53          |
| (1,119)  | 1:A:77:VAL:HB   | 1:A:146:ASP:HB3  | 1        | 1.53          |
| (1,1032) | 1:B:81:VAL:HG21 | 1:B:118:PHE:HD1  | 3        | 1.53          |
| (1,1032) | 1:B:81:VAL:HG21 | 1:B:118:PHE:HD2  | 3        | 1.53          |
| (1,1032) | 1:B:81:VAL:HG22 | 1:B:118:PHE:HD1  | 3        | 1.53          |
| (1,1032) | 1:B:81:VAL:HG22 | 1:B:118:PHE:HD2  | 3        | 1.53          |
| (1,1032) | 1:B:81:VAL:HG23 | 1:B:118:PHE:HD1  | 3        | 1.53          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1032) | 1:B:81:VAL:HG23 | 1:B:118:PHE:HD2  | 3        | 1.53          |
| (1,258)  | 1:A:89:LEU:HD11 | 1:A:102:GLY:HA2  | 1        | 1.52          |
| (1,258)  | 1:A:89:LEU:HD12 | 1:A:102:GLY:HA2  | 1        | 1.52          |
| (1,258)  | 1:A:89:LEU:HD13 | 1:A:102:GLY:HA2  | 1        | 1.52          |
| (1,257)  | 1:A:89:LEU:HD11 | 1:A:102:GLY:HA2  | 1        | 1.52          |
| (1,257)  | 1:A:89:LEU:HD12 | 1:A:102:GLY:HA2  | 1        | 1.52          |
| (1,257)  | 1:A:89:LEU:HD13 | 1:A:102:GLY:HA2  | 1        | 1.52          |
| (1,1125) | 1:B:89:LEU:HD11 | 1:B:102:GLY:HA2  | 1        | 1.52          |
| (1,1125) | 1:B:89:LEU:HD12 | 1:B:102:GLY:HA2  | 1        | 1.52          |
| (1,1125) | 1:B:89:LEU:HD13 | 1:B:102:GLY:HA2  | 1        | 1.52          |
| (1,1124) | 1:B:89:LEU:HD11 | 1:B:102:GLY:HA2  | 1        | 1.52          |
| (1,1124) | 1:B:89:LEU:HD12 | 1:B:102:GLY:HA2  | 1        | 1.52          |
| (1,1124) | 1:B:89:LEU:HD13 | 1:B:102:GLY:HA2  | 1        | 1.52          |
| (1,702)  | 1:A:132:THR:HB  | 1:A:133:ILE:HG12 | 9        | 1.51          |
| (1,702)  | 1:A:132:THR:HB  | 1:A:133:ILE:HG13 | 9        | 1.51          |
| (1,555)  | 1:A:118:PHE:HB2 | 1:A:117:GLU:H    | 1        | 1.51          |
| (1,258)  | 1:A:89:LEU:HD11 | 1:A:102:GLY:HA2  | 3        | 1.51          |
| (1,258)  | 1:A:89:LEU:HD12 | 1:A:102:GLY:HA2  | 3        | 1.51          |
| (1,258)  | 1:A:89:LEU:HD13 | 1:A:102:GLY:HA2  | 3        | 1.51          |
| (1,257)  | 1:A:89:LEU:HD11 | 1:A:102:GLY:HA2  | 3        | 1.51          |
| (1,257)  | 1:A:89:LEU:HD12 | 1:A:102:GLY:HA2  | 3        | 1.51          |
| (1,257)  | 1:A:89:LEU:HD13 | 1:A:102:GLY:HA2  | 3        | 1.51          |
| (1,254)  | 1:A:89:LEU:HD11 | 1:A:91:VAL:HB    | 1        | 1.51          |
| (1,254)  | 1:A:89:LEU:HD12 | 1:A:91:VAL:HB    | 1        | 1.51          |
| (1,254)  | 1:A:89:LEU:HD13 | 1:A:91:VAL:HB    | 1        | 1.51          |
| (1,187)  | 1:A:83:HIS:HB3  | 1:A:104:HIS:HD2  | 6        | 1.51          |
| (1,1569) | 1:B:132:THR:HB  | 1:B:133:ILE:HG12 | 9        | 1.51          |
| (1,1569) | 1:B:132:THR:HB  | 1:B:133:ILE:HG13 | 9        | 1.51          |
| (1,1422) | 1:B:118:PHE:HB2 | 1:B:117:GLU:H    | 1        | 1.51          |
| (1,1125) | 1:B:89:LEU:HD11 | 1:B:102:GLY:HA2  | 3        | 1.51          |
| (1,1125) | 1:B:89:LEU:HD12 | 1:B:102:GLY:HA2  | 3        | 1.51          |
| (1,1125) | 1:B:89:LEU:HD13 | 1:B:102:GLY:HA2  | 3        | 1.51          |
| (1,1124) | 1:B:89:LEU:HD11 | 1:B:102:GLY:HA2  | 3        | 1.51          |
| (1,1124) | 1:B:89:LEU:HD12 | 1:B:102:GLY:HA2  | 3        | 1.51          |
| (1,1124) | 1:B:89:LEU:HD13 | 1:B:102:GLY:HA2  | 3        | 1.51          |
| (1,1121) | 1:B:89:LEU:HD11 | 1:B:91:VAL:HB    | 1        | 1.51          |
| (1,1121) | 1:B:89:LEU:HD12 | 1:B:91:VAL:HB    | 1        | 1.51          |
| (1,1121) | 1:B:89:LEU:HD13 | 1:B:91:VAL:HB    | 1        | 1.51          |
| (1,1054) | 1:B:83:HIS:HB3  | 1:B:104:HIS:HD2  | 6        | 1.51          |
| (1,985)  | 1:B:77:VAL:HB   | 1:B:146:ASP:HB2  | 2        | 1.5           |
| (1,642)  | 1:A:125:PRO:HD3 | 1:A:122:TYR:HD1  | 5        | 1.5           |
| (1,642)  | 1:A:125:PRO:HD3 | 1:A:122:TYR:HD2  | 5        | 1.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,188)  | 1:A:83:HIS:H     | 1:A:141:GLY:HA2  | 1        | 1.5           |
| (1,1509) | 1:B:125:PRO:HD3  | 1:B:122:TYR:HD1  | 5        | 1.5           |
| (1,1509) | 1:B:125:PRO:HD3  | 1:B:122:TYR:HD2  | 5        | 1.5           |
| (1,118)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB2  | 2        | 1.5           |
| (1,118)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB2  | 5        | 1.5           |
| (1,1055) | 1:B:83:HIS:H     | 1:B:141:GLY:HA2  | 1        | 1.5           |
| (1,985)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB2  | 5        | 1.49          |
| (1,555)  | 1:A:118:PHE:HB2  | 1:A:117:GLU:H    | 8        | 1.49          |
| (1,497)  | 1:A:113:PHE:HD1  | 1:A:113:PHE:H    | 5        | 1.49          |
| (1,497)  | 1:A:113:PHE:HD2  | 1:A:113:PHE:H    | 5        | 1.49          |
| (1,481)  | 1:A:113:PHE:HA   | 1:A:107:ARG:HB2  | 6        | 1.49          |
| (1,426)  | 1:A:107:ARG:HD2  | 1:A:107:ARG:H    | 4        | 1.49          |
| (1,238)  | 1:A:89:LEU:HD11  | 1:A:85:SER:H     | 5        | 1.49          |
| (1,238)  | 1:A:89:LEU:HD12  | 1:A:85:SER:H     | 5        | 1.49          |
| (1,238)  | 1:A:89:LEU:HD13  | 1:A:85:SER:H     | 5        | 1.49          |
| (1,188)  | 1:A:83:HIS:H     | 1:A:141:GLY:HA2  | 7        | 1.49          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG12 | 9        | 1.49          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG13 | 9        | 1.49          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD1  | 5        | 1.49          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD2  | 5        | 1.49          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD1  | 5        | 1.49          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD2  | 5        | 1.49          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD1  | 5        | 1.49          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD2  | 5        | 1.49          |
| (1,1422) | 1:B:118:PHE:HB2  | 1:B:117:GLU:H    | 8        | 1.49          |
| (1,1364) | 1:B:113:PHE:HD1  | 1:B:113:PHE:H    | 5        | 1.49          |
| (1,1364) | 1:B:113:PHE:HD2  | 1:B:113:PHE:H    | 5        | 1.49          |
| (1,1348) | 1:B:113:PHE:HA   | 1:B:107:ARG:HB2  | 6        | 1.49          |
| (1,1293) | 1:B:107:ARG:HD2  | 1:B:107:ARG:H    | 4        | 1.49          |
| (1,1105) | 1:B:89:LEU:HD11  | 1:B:85:SER:H     | 5        | 1.49          |
| (1,1105) | 1:B:89:LEU:HD12  | 1:B:85:SER:H     | 5        | 1.49          |
| (1,1105) | 1:B:89:LEU:HD13  | 1:B:85:SER:H     | 5        | 1.49          |
| (1,1055) | 1:B:83:HIS:H     | 1:B:141:GLY:HA2  | 7        | 1.49          |
| (1,506)  | 1:A:114:ILE:HB   | 1:A:107:ARG:HD3  | 3        | 1.48          |
| (1,421)  | 1:A:107:ARG:HD2  | 1:A:105:GLU:H    | 8        | 1.48          |
| (1,188)  | 1:A:83:HIS:H     | 1:A:141:GLY:HA2  | 6        | 1.48          |
| (1,1373) | 1:B:114:ILE:HB   | 1:B:107:ARG:HD3  | 3        | 1.48          |
| (1,1288) | 1:B:107:ARG:HD2  | 1:B:105:GLU:H    | 8        | 1.48          |
| (1,1055) | 1:B:83:HIS:H     | 1:B:141:GLY:HA2  | 6        | 1.48          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD11  | 5        | 1.47          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD12  | 5        | 1.47          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD13  | 5        | 1.47          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,919)  | 1:B:75:PHE:HE2  | 1:B:98:ILE:HD11  | 5        | 1.47          |
| (1,919)  | 1:B:75:PHE:HE2  | 1:B:98:ILE:HD12  | 5        | 1.47          |
| (1,919)  | 1:B:75:PHE:HE2  | 1:B:98:ILE:HD13  | 5        | 1.47          |
| (1,912)  | 1:B:75:PHE:HA   | 1:B:74:ARG:HG2   | 6        | 1.47          |
| (1,912)  | 1:B:75:PHE:HA   | 1:B:74:ARG:HG3   | 6        | 1.47          |
| (1,52)   | 1:A:75:PHE:HE1  | 1:A:98:ILE:HD11  | 5        | 1.47          |
| (1,52)   | 1:A:75:PHE:HE1  | 1:A:98:ILE:HD12  | 5        | 1.47          |
| (1,52)   | 1:A:75:PHE:HE1  | 1:A:98:ILE:HD13  | 5        | 1.47          |
| (1,52)   | 1:A:75:PHE:HE2  | 1:A:98:ILE:HD11  | 5        | 1.47          |
| (1,52)   | 1:A:75:PHE:HE2  | 1:A:98:ILE:HD12  | 5        | 1.47          |
| (1,52)   | 1:A:75:PHE:HE2  | 1:A:98:ILE:HD13  | 5        | 1.47          |
| (1,481)  | 1:A:113:PHE:HA  | 1:A:107:ARG:HB2  | 1        | 1.47          |
| (1,45)   | 1:A:75:PHE:HA   | 1:A:74:ARG:HG2   | 6        | 1.47          |
| (1,45)   | 1:A:75:PHE:HA   | 1:A:74:ARG:HG3   | 6        | 1.47          |
| (1,1754) | 1:A:118:PHE:HZ  | 1:B:116:ARG:HA   | 6        | 1.47          |
| (1,1470) | 1:B:122:TYR:HA  | 1:B:124:ILE:HD11 | 7        | 1.47          |
| (1,1470) | 1:B:122:TYR:HA  | 1:B:124:ILE:HD12 | 7        | 1.47          |
| (1,1470) | 1:B:122:TYR:HA  | 1:B:124:ILE:HD13 | 7        | 1.47          |
| (1,1348) | 1:B:113:PHE:HA  | 1:B:107:ARG:HB2  | 1        | 1.47          |
| (1,971)  | 1:B:77:VAL:HG21 | 1:B:79:LEU:HB2   | 4        | 1.46          |
| (1,971)  | 1:B:77:VAL:HG21 | 1:B:79:LEU:HB3   | 4        | 1.46          |
| (1,971)  | 1:B:77:VAL:HG22 | 1:B:79:LEU:HB2   | 4        | 1.46          |
| (1,971)  | 1:B:77:VAL:HG22 | 1:B:79:LEU:HB3   | 4        | 1.46          |
| (1,971)  | 1:B:77:VAL:HG23 | 1:B:79:LEU:HB2   | 4        | 1.46          |
| (1,971)  | 1:B:77:VAL:HG23 | 1:B:79:LEU:HB3   | 4        | 1.46          |
| (1,603)  | 1:A:122:TYR:HA  | 1:A:124:ILE:HD11 | 7        | 1.46          |
| (1,603)  | 1:A:122:TYR:HA  | 1:A:124:ILE:HD12 | 7        | 1.46          |
| (1,603)  | 1:A:122:TYR:HA  | 1:A:124:ILE:HD13 | 7        | 1.46          |
| (1,1311) | 1:B:108:GLN:HA  | 1:B:113:PHE:HE1  | 7        | 1.46          |
| (1,1311) | 1:B:108:GLN:HA  | 1:B:113:PHE:HE2  | 7        | 1.46          |
| (1,104)  | 1:A:77:VAL:HG21 | 1:A:79:LEU:HB2   | 4        | 1.46          |
| (1,104)  | 1:A:77:VAL:HG21 | 1:A:79:LEU:HB3   | 4        | 1.46          |
| (1,104)  | 1:A:77:VAL:HG22 | 1:A:79:LEU:HB2   | 4        | 1.46          |
| (1,104)  | 1:A:77:VAL:HG22 | 1:A:79:LEU:HB3   | 4        | 1.46          |
| (1,104)  | 1:A:77:VAL:HG23 | 1:A:79:LEU:HB2   | 4        | 1.46          |
| (1,104)  | 1:A:77:VAL:HG23 | 1:A:79:LEU:HB3   | 4        | 1.46          |
| (1,893)  | 1:B:71:GLU:H    | 1:B:76:SER:H     | 3        | 1.45          |
| (1,813)  | 1:A:145:VAL:HA  | 1:A:135:SER:H    | 8        | 1.45          |
| (1,53)   | 1:A:75:PHE:HE1  | 1:A:133:ILE:HD11 | 9        | 1.45          |
| (1,53)   | 1:A:75:PHE:HE1  | 1:A:133:ILE:HD12 | 9        | 1.45          |
| (1,53)   | 1:A:75:PHE:HE1  | 1:A:133:ILE:HD13 | 9        | 1.45          |
| (1,53)   | 1:A:75:PHE:HE2  | 1:A:133:ILE:HD11 | 9        | 1.45          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,53)   | 1:A:75:PHE:HE2  | 1:A:133:ILE:HD12 | 9        | 1.45          |
| (1,53)   | 1:A:75:PHE:HE2  | 1:A:133:ILE:HD13 | 9        | 1.45          |
| (1,483)  | 1:A:113:PHE:HE1 | 1:A:107:ARG:HA   | 7        | 1.45          |
| (1,483)  | 1:A:113:PHE:HE2 | 1:A:107:ARG:HA   | 7        | 1.45          |
| (1,444)  | 1:A:108:GLN:HA  | 1:A:113:PHE:HE1  | 7        | 1.45          |
| (1,444)  | 1:A:108:GLN:HA  | 1:A:113:PHE:HE2  | 7        | 1.45          |
| (1,26)   | 1:A:71:GLU:H    | 1:A:76:SER:H     | 3        | 1.45          |
| (1,186)  | 1:A:83:HIS:HB2  | 1:A:104:HIS:HB2  | 3        | 1.45          |
| (1,1680) | 1:B:145:VAL:HA  | 1:B:135:SER:H    | 8        | 1.45          |
| (1,1350) | 1:B:113:PHE:HE1 | 1:B:107:ARG:HA   | 7        | 1.45          |
| (1,1350) | 1:B:113:PHE:HE2 | 1:B:107:ARG:HA   | 7        | 1.45          |
| (1,1054) | 1:B:83:HIS:HB3  | 1:B:104:HIS:HD2  | 5        | 1.45          |
| (1,1053) | 1:B:83:HIS:HB2  | 1:B:104:HIS:HB2  | 3        | 1.45          |
| (1,920)  | 1:B:75:PHE:HE1  | 1:B:133:ILE:HD11 | 9        | 1.44          |
| (1,920)  | 1:B:75:PHE:HE1  | 1:B:133:ILE:HD12 | 9        | 1.44          |
| (1,920)  | 1:B:75:PHE:HE1  | 1:B:133:ILE:HD13 | 9        | 1.44          |
| (1,920)  | 1:B:75:PHE:HE2  | 1:B:133:ILE:HD11 | 9        | 1.44          |
| (1,920)  | 1:B:75:PHE:HE2  | 1:B:133:ILE:HD12 | 9        | 1.44          |
| (1,920)  | 1:B:75:PHE:HE2  | 1:B:133:ILE:HD13 | 9        | 1.44          |
| (1,880)  | 1:B:68:MET:HE1  | 1:B:122:TYR:HE1  | 4        | 1.44          |
| (1,880)  | 1:B:68:MET:HE1  | 1:B:122:TYR:HE2  | 4        | 1.44          |
| (1,880)  | 1:B:68:MET:HE2  | 1:B:122:TYR:HE1  | 4        | 1.44          |
| (1,880)  | 1:B:68:MET:HE2  | 1:B:122:TYR:HE2  | 4        | 1.44          |
| (1,880)  | 1:B:68:MET:HE3  | 1:B:122:TYR:HE1  | 4        | 1.44          |
| (1,880)  | 1:B:68:MET:HE3  | 1:B:122:TYR:HE2  | 4        | 1.44          |
| (1,702)  | 1:A:132:THR:HB  | 1:A:133:ILE:HG12 | 8        | 1.44          |
| (1,702)  | 1:A:132:THR:HB  | 1:A:133:ILE:HG13 | 8        | 1.44          |
| (1,595)  | 1:A:122:TYR:HD1 | 1:A:122:TYR:H    | 5        | 1.44          |
| (1,595)  | 1:A:122:TYR:HD2 | 1:A:122:TYR:H    | 5        | 1.44          |
| (1,564)  | 1:A:118:PHE:HD1 | 1:A:118:PHE:H    | 8        | 1.44          |
| (1,564)  | 1:A:118:PHE:HD2 | 1:A:118:PHE:H    | 8        | 1.44          |
| (1,187)  | 1:A:83:HIS:HB3  | 1:A:104:HIS:HD2  | 5        | 1.44          |
| (1,1569) | 1:B:132:THR:HB  | 1:B:133:ILE:HG12 | 8        | 1.44          |
| (1,1569) | 1:B:132:THR:HB  | 1:B:133:ILE:HG13 | 8        | 1.44          |
| (1,13)   | 1:A:68:MET:HE1  | 1:A:122:TYR:HE1  | 4        | 1.44          |
| (1,13)   | 1:A:68:MET:HE1  | 1:A:122:TYR:HE2  | 4        | 1.44          |
| (1,13)   | 1:A:68:MET:HE2  | 1:A:122:TYR:HE1  | 4        | 1.44          |
| (1,13)   | 1:A:68:MET:HE2  | 1:A:122:TYR:HE2  | 4        | 1.44          |
| (1,13)   | 1:A:68:MET:HE3  | 1:A:122:TYR:HE1  | 4        | 1.44          |
| (1,13)   | 1:A:68:MET:HE3  | 1:A:122:TYR:HE2  | 4        | 1.44          |
| (1,951)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE1   | 4        | 1.43          |
| (1,951)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE2   | 4        | 1.43          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,951) | 1:B:77:VAL:HG21  | 1:B:68:MET:HE3  | 4        | 1.43          |
| (1,951) | 1:B:77:VAL:HG22  | 1:B:68:MET:HE1  | 4        | 1.43          |
| (1,951) | 1:B:77:VAL:HG22  | 1:B:68:MET:HE2  | 4        | 1.43          |
| (1,951) | 1:B:77:VAL:HG22  | 1:B:68:MET:HE3  | 4        | 1.43          |
| (1,951) | 1:B:77:VAL:HG23  | 1:B:68:MET:HE1  | 4        | 1.43          |
| (1,951) | 1:B:77:VAL:HG23  | 1:B:68:MET:HE2  | 4        | 1.43          |
| (1,951) | 1:B:77:VAL:HG23  | 1:B:68:MET:HE3  | 4        | 1.43          |
| (1,946) | 1:B:77:VAL:HG21  | 1:B:68:MET:HE1  | 4        | 1.43          |
| (1,946) | 1:B:77:VAL:HG21  | 1:B:68:MET:HE2  | 4        | 1.43          |
| (1,946) | 1:B:77:VAL:HG21  | 1:B:68:MET:HE3  | 4        | 1.43          |
| (1,946) | 1:B:77:VAL:HG22  | 1:B:68:MET:HE1  | 4        | 1.43          |
| (1,946) | 1:B:77:VAL:HG22  | 1:B:68:MET:HE2  | 4        | 1.43          |
| (1,946) | 1:B:77:VAL:HG22  | 1:B:68:MET:HE3  | 4        | 1.43          |
| (1,946) | 1:B:77:VAL:HG23  | 1:B:68:MET:HE1  | 4        | 1.43          |
| (1,946) | 1:B:77:VAL:HG23  | 1:B:68:MET:HE2  | 4        | 1.43          |
| (1,946) | 1:B:77:VAL:HG23  | 1:B:68:MET:HE3  | 4        | 1.43          |
| (1,912) | 1:B:75:PHE:HA    | 1:B:74:ARG:HG2  | 3        | 1.43          |
| (1,912) | 1:B:75:PHE:HA    | 1:B:74:ARG:HG3  | 3        | 1.43          |
| (1,84)  | 1:A:77:VAL:HG21  | 1:A:68:MET:HE1  | 4        | 1.43          |
| (1,84)  | 1:A:77:VAL:HG21  | 1:A:68:MET:HE2  | 4        | 1.43          |
| (1,84)  | 1:A:77:VAL:HG21  | 1:A:68:MET:HE3  | 4        | 1.43          |
| (1,84)  | 1:A:77:VAL:HG22  | 1:A:68:MET:HE1  | 4        | 1.43          |
| (1,84)  | 1:A:77:VAL:HG22  | 1:A:68:MET:HE2  | 4        | 1.43          |
| (1,84)  | 1:A:77:VAL:HG22  | 1:A:68:MET:HE3  | 4        | 1.43          |
| (1,84)  | 1:A:77:VAL:HG23  | 1:A:68:MET:HE1  | 4        | 1.43          |
| (1,84)  | 1:A:77:VAL:HG23  | 1:A:68:MET:HE2  | 4        | 1.43          |
| (1,84)  | 1:A:77:VAL:HG23  | 1:A:68:MET:HE3  | 4        | 1.43          |
| (1,79)  | 1:A:77:VAL:HG21  | 1:A:68:MET:HE1  | 4        | 1.43          |
| (1,79)  | 1:A:77:VAL:HG21  | 1:A:68:MET:HE2  | 4        | 1.43          |
| (1,79)  | 1:A:77:VAL:HG21  | 1:A:68:MET:HE3  | 4        | 1.43          |
| (1,79)  | 1:A:77:VAL:HG22  | 1:A:68:MET:HE1  | 4        | 1.43          |
| (1,79)  | 1:A:77:VAL:HG22  | 1:A:68:MET:HE2  | 4        | 1.43          |
| (1,79)  | 1:A:77:VAL:HG22  | 1:A:68:MET:HE3  | 4        | 1.43          |
| (1,79)  | 1:A:77:VAL:HG23  | 1:A:68:MET:HE1  | 4        | 1.43          |
| (1,79)  | 1:A:77:VAL:HG23  | 1:A:68:MET:HE2  | 4        | 1.43          |
| (1,79)  | 1:A:77:VAL:HG23  | 1:A:68:MET:HE3  | 4        | 1.43          |
| (1,605) | 1:A:123:ARG:HD2  | 1:A:98:ILE:H    | 5        | 1.43          |
| (1,605) | 1:A:123:ARG:HD3  | 1:A:98:ILE:H    | 5        | 1.43          |
| (1,525) | 1:A:115:SER:HB3  | 1:A:107:ARG:H   | 5        | 1.43          |
| (1,502) | 1:A:114:ILE:HD11 | 1:A:104:HIS:HB2 | 9        | 1.43          |
| (1,502) | 1:A:114:ILE:HD12 | 1:A:104:HIS:HB2 | 9        | 1.43          |
| (1,502) | 1:A:114:ILE:HD13 | 1:A:104:HIS:HB2 | 9        | 1.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,481)  | 1:A:113:PHE:HA   | 1:A:107:ARG:HB2  | 2        | 1.43          |
| (1,45)   | 1:A:75:PHE:HA    | 1:A:74:ARG:HG2   | 3        | 1.43          |
| (1,45)   | 1:A:75:PHE:HA    | 1:A:74:ARG:HG3   | 3        | 1.43          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD1  | 6        | 1.43          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD2  | 6        | 1.43          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD1  | 6        | 1.43          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD2  | 6        | 1.43          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD1  | 6        | 1.43          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD2  | 6        | 1.43          |
| (1,1472) | 1:B:123:ARG:HD2  | 1:B:98:ILE:H     | 5        | 1.43          |
| (1,1472) | 1:B:123:ARG:HD3  | 1:B:98:ILE:H     | 5        | 1.43          |
| (1,1462) | 1:B:122:TYR:HD1  | 1:B:122:TYR:H    | 5        | 1.43          |
| (1,1462) | 1:B:122:TYR:HD2  | 1:B:122:TYR:H    | 5        | 1.43          |
| (1,1431) | 1:B:118:PHE:HD1  | 1:B:118:PHE:H    | 8        | 1.43          |
| (1,1431) | 1:B:118:PHE:HD2  | 1:B:118:PHE:H    | 8        | 1.43          |
| (1,1392) | 1:B:115:SER:HB3  | 1:B:107:ARG:H    | 5        | 1.43          |
| (1,1369) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HB2  | 9        | 1.43          |
| (1,1369) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HB2  | 9        | 1.43          |
| (1,1369) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HB2  | 9        | 1.43          |
| (1,1348) | 1:B:113:PHE:HA   | 1:B:107:ARG:HB2  | 2        | 1.43          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG11 | 3        | 1.43          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG12 | 3        | 1.43          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG13 | 3        | 1.43          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG11 | 3        | 1.43          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG12 | 3        | 1.43          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG13 | 3        | 1.43          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG11 | 3        | 1.43          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG12 | 3        | 1.43          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG13 | 3        | 1.43          |
| (1,813)  | 1:A:145:VAL:HA   | 1:A:135:SER:H    | 4        | 1.42          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD11 | 8        | 1.42          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD12 | 8        | 1.42          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD13 | 8        | 1.42          |
| (1,502)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HB2  | 6        | 1.42          |
| (1,502)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HB2  | 6        | 1.42          |
| (1,502)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HB2  | 6        | 1.42          |
| (1,321)  | 1:A:97:VAL:H     | 1:A:93:VAL:HB    | 6        | 1.42          |
| (1,203)  | 1:A:84:PHE:HE1   | 1:A:116:ARG:H    | 1        | 1.42          |
| (1,203)  | 1:A:84:PHE:HE2   | 1:A:116:ARG:H    | 1        | 1.42          |
| (1,190)  | 1:A:84:PHE:HE1   | 1:A:82:LYS:H     | 7        | 1.42          |
| (1,190)  | 1:A:84:PHE:HE2   | 1:A:82:LYS:H     | 7        | 1.42          |
| (1,1680) | 1:B:145:VAL:HA   | 1:B:135:SER:H    | 4        | 1.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD11 | 8        | 1.42          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD12 | 8        | 1.42          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD13 | 8        | 1.42          |
| (1,1188) | 1:B:97:VAL:H     | 1:B:93:VAL:HB    | 6        | 1.42          |
| (1,1070) | 1:B:84:PHE:HE1   | 1:B:116:ARG:H    | 1        | 1.42          |
| (1,1070) | 1:B:84:PHE:HE2   | 1:B:116:ARG:H    | 1        | 1.42          |
| (1,1057) | 1:B:84:PHE:HE1   | 1:B:82:LYS:H     | 7        | 1.42          |
| (1,1057) | 1:B:84:PHE:HE2   | 1:B:82:LYS:H     | 7        | 1.42          |
| (1,981)  | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG11 | 3        | 1.41          |
| (1,981)  | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG12 | 3        | 1.41          |
| (1,981)  | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG13 | 3        | 1.41          |
| (1,981)  | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG11 | 3        | 1.41          |
| (1,981)  | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG12 | 3        | 1.41          |
| (1,981)  | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG13 | 3        | 1.41          |
| (1,981)  | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG11 | 3        | 1.41          |
| (1,981)  | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG12 | 3        | 1.41          |
| (1,981)  | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG13 | 3        | 1.41          |
| (1,1369) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HB2  | 6        | 1.41          |
| (1,1369) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HB2  | 6        | 1.41          |
| (1,1369) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HB2  | 6        | 1.41          |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB2   | 2        | 1.4           |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB3   | 2        | 1.4           |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB2   | 2        | 1.4           |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB3   | 2        | 1.4           |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB2   | 2        | 1.4           |
| (1,971)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB3   | 2        | 1.4           |
| (1,906)  | 1:B:74:ARG:HG2   | 1:B:73:ASP:H     | 2        | 1.4           |
| (1,906)  | 1:B:74:ARG:HG3   | 1:B:73:ASP:H     | 2        | 1.4           |
| (1,887)  | 1:B:70:LEU:HB3   | 1:B:71:GLU:H     | 7        | 1.4           |
| (1,619)  | 1:A:124:ILE:HA   | 1:A:122:TYR:HD1  | 9        | 1.4           |
| (1,619)  | 1:A:124:ILE:HA   | 1:A:122:TYR:HD2  | 9        | 1.4           |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD11 | 3        | 1.4           |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD12 | 3        | 1.4           |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD13 | 3        | 1.4           |
| (1,483)  | 1:A:113:PHE:HE1  | 1:A:107:ARG:HA   | 5        | 1.4           |
| (1,483)  | 1:A:113:PHE:HE2  | 1:A:107:ARG:HA   | 5        | 1.4           |
| (1,39)   | 1:A:74:ARG:HG2   | 1:A:73:ASP:H     | 2        | 1.4           |
| (1,39)   | 1:A:74:ARG:HG3   | 1:A:73:ASP:H     | 2        | 1.4           |
| (1,342)  | 1:A:98:ILE:HD11  | 1:A:122:TYR:HD1  | 2        | 1.4           |
| (1,342)  | 1:A:98:ILE:HD11  | 1:A:122:TYR:HD2  | 2        | 1.4           |
| (1,342)  | 1:A:98:ILE:HD12  | 1:A:122:TYR:HD1  | 2        | 1.4           |
| (1,342)  | 1:A:98:ILE:HD12  | 1:A:122:TYR:HD2  | 2        | 1.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,342)  | 1:A:98:ILE:HD13  | 1:A:122:TYR:HD1  | 2        | 1.4           |
| (1,342)  | 1:A:98:ILE:HD13  | 1:A:122:TYR:HD2  | 2        | 1.4           |
| (1,20)   | 1:A:70:LEU:HB3   | 1:A:71:GLU:H     | 7        | 1.4           |
| (1,1486) | 1:B:124:ILE:HA   | 1:B:122:TYR:HD1  | 9        | 1.4           |
| (1,1486) | 1:B:124:ILE:HA   | 1:B:122:TYR:HD2  | 9        | 1.4           |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD11 | 3        | 1.4           |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD12 | 3        | 1.4           |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD13 | 3        | 1.4           |
| (1,1350) | 1:B:113:PHE:HE1  | 1:B:107:ARG:HA   | 5        | 1.4           |
| (1,1350) | 1:B:113:PHE:HE2  | 1:B:107:ARG:HA   | 5        | 1.4           |
| (1,1209) | 1:B:98:ILE:HD11  | 1:B:122:TYR:HD1  | 2        | 1.4           |
| (1,1209) | 1:B:98:ILE:HD11  | 1:B:122:TYR:HD2  | 2        | 1.4           |
| (1,1209) | 1:B:98:ILE:HD12  | 1:B:122:TYR:HD1  | 2        | 1.4           |
| (1,1209) | 1:B:98:ILE:HD12  | 1:B:122:TYR:HD2  | 2        | 1.4           |
| (1,1209) | 1:B:98:ILE:HD13  | 1:B:122:TYR:HD1  | 2        | 1.4           |
| (1,1209) | 1:B:98:ILE:HD13  | 1:B:122:TYR:HD2  | 2        | 1.4           |
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB2   | 2        | 1.4           |
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB3   | 2        | 1.4           |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB2   | 2        | 1.4           |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB3   | 2        | 1.4           |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB2   | 2        | 1.4           |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB3   | 2        | 1.4           |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG12 | 5        | 1.39          |
| (1,702)  | 1:A:132:THR:HB   | 1:A:133:ILE:HG13 | 5        | 1.39          |
| (1,641)  | 1:A:124:ILE:HG21 | 1:A:148:PRO:HA   | 4        | 1.39          |
| (1,641)  | 1:A:124:ILE:HG22 | 1:A:148:PRO:HA   | 4        | 1.39          |
| (1,641)  | 1:A:124:ILE:HG23 | 1:A:148:PRO:HA   | 4        | 1.39          |
| (1,195)  | 1:A:84:PHE:HD1   | 1:A:84:PHE:H     | 3        | 1.39          |
| (1,195)  | 1:A:84:PHE:HD2   | 1:A:84:PHE:H     | 3        | 1.39          |
| (1,1745) | 1:A:114:ILE:H    | 1:B:121:LYS:H    | 7        | 1.39          |
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG12 | 5        | 1.39          |
| (1,1569) | 1:B:132:THR:HB   | 1:B:133:ILE:HG13 | 5        | 1.39          |
| (1,1508) | 1:B:124:ILE:HG21 | 1:B:148:PRO:HA   | 4        | 1.39          |
| (1,1508) | 1:B:124:ILE:HG22 | 1:B:148:PRO:HA   | 4        | 1.39          |
| (1,1508) | 1:B:124:ILE:HG23 | 1:B:148:PRO:HA   | 4        | 1.39          |
| (1,1062) | 1:B:84:PHE:HD1   | 1:B:84:PHE:H     | 3        | 1.39          |
| (1,1062) | 1:B:84:PHE:HD2   | 1:B:84:PHE:H     | 3        | 1.39          |
| (1,481)  | 1:A:113:PHE:HA   | 1:A:107:ARG:HB2  | 7        | 1.38          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD11 | 2        | 1.38          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD12 | 2        | 1.38          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD13 | 2        | 1.38          |
| (1,1348) | 1:B:113:PHE:HA   | 1:B:107:ARG:HB2  | 7        | 1.38          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,98)   | 1:A:77:VAL:HG11 | 1:A:77:VAL:H     | 6        | 1.37          |
| (1,98)   | 1:A:77:VAL:HG12 | 1:A:77:VAL:H     | 6        | 1.37          |
| (1,98)   | 1:A:77:VAL:HG13 | 1:A:77:VAL:H     | 6        | 1.37          |
| (1,965)  | 1:B:77:VAL:HG11 | 1:B:77:VAL:H     | 6        | 1.37          |
| (1,965)  | 1:B:77:VAL:HG12 | 1:B:77:VAL:H     | 6        | 1.37          |
| (1,965)  | 1:B:77:VAL:HG13 | 1:B:77:VAL:H     | 6        | 1.37          |
| (1,603)  | 1:A:122:TYR:HA  | 1:A:124:ILE:HD11 | 2        | 1.37          |
| (1,603)  | 1:A:122:TYR:HA  | 1:A:124:ILE:HD12 | 2        | 1.37          |
| (1,603)  | 1:A:122:TYR:HA  | 1:A:124:ILE:HD13 | 2        | 1.37          |
| (1,1422) | 1:B:118:PHE:HB2 | 1:B:117:GLU:H    | 2        | 1.37          |
| (1,951)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE1   | 2        | 1.36          |
| (1,951)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE2   | 2        | 1.36          |
| (1,951)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE3   | 2        | 1.36          |
| (1,951)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE1   | 2        | 1.36          |
| (1,951)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE2   | 2        | 1.36          |
| (1,951)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE3   | 2        | 1.36          |
| (1,951)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE1   | 2        | 1.36          |
| (1,951)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE2   | 2        | 1.36          |
| (1,951)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE3   | 2        | 1.36          |
| (1,946)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE1   | 2        | 1.36          |
| (1,946)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE2   | 2        | 1.36          |
| (1,946)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE3   | 2        | 1.36          |
| (1,946)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE1   | 2        | 1.36          |
| (1,946)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE2   | 2        | 1.36          |
| (1,946)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE3   | 2        | 1.36          |
| (1,946)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE1   | 2        | 1.36          |
| (1,946)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE2   | 2        | 1.36          |
| (1,946)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE3   | 2        | 1.36          |
| (1,906)  | 1:B:74:ARG:HG2  | 1:B:73:ASP:H     | 1        | 1.36          |
| (1,906)  | 1:B:74:ARG:HG3  | 1:B:73:ASP:H     | 1        | 1.36          |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG21 | 4        | 1.36          |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG22 | 4        | 1.36          |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG23 | 4        | 1.36          |
| (1,555)  | 1:A:118:PHE:HB2 | 1:A:117:GLU:H    | 2        | 1.36          |
| (1,522)  | 1:A:115:SER:HB3 | 1:A:105:GLU:HB2  | 1        | 1.36          |
| (1,522)  | 1:A:115:SER:HB3 | 1:A:105:GLU:HB3  | 1        | 1.36          |
| (1,39)   | 1:A:74:ARG:HG2  | 1:A:73:ASP:H     | 1        | 1.36          |
| (1,39)   | 1:A:74:ARG:HG3  | 1:A:73:ASP:H     | 1        | 1.36          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG21 | 4        | 1.36          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG22 | 4        | 1.36          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG23 | 4        | 1.36          |
| (1,1389) | 1:B:115:SER:HB3 | 1:B:105:GLU:HB2  | 1        | 1.36          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB3 | 1        | 1.36          |
| (1,1348) | 1:B:113:PHE:HA   | 1:B:107:ARG:HB2 | 8        | 1.36          |
| (1,912)  | 1:B:75:PHE:HA    | 1:B:74:ARG:HG2  | 9        | 1.35          |
| (1,912)  | 1:B:75:PHE:HA    | 1:B:74:ARG:HG3  | 9        | 1.35          |
| (1,84)   | 1:A:77:VAL:HG21  | 1:A:68:MET:HE1  | 2        | 1.35          |
| (1,84)   | 1:A:77:VAL:HG21  | 1:A:68:MET:HE2  | 2        | 1.35          |
| (1,84)   | 1:A:77:VAL:HG21  | 1:A:68:MET:HE3  | 2        | 1.35          |
| (1,84)   | 1:A:77:VAL:HG22  | 1:A:68:MET:HE1  | 2        | 1.35          |
| (1,84)   | 1:A:77:VAL:HG22  | 1:A:68:MET:HE2  | 2        | 1.35          |
| (1,84)   | 1:A:77:VAL:HG22  | 1:A:68:MET:HE3  | 2        | 1.35          |
| (1,84)   | 1:A:77:VAL:HG23  | 1:A:68:MET:HE1  | 2        | 1.35          |
| (1,84)   | 1:A:77:VAL:HG23  | 1:A:68:MET:HE2  | 2        | 1.35          |
| (1,84)   | 1:A:77:VAL:HG23  | 1:A:68:MET:HE3  | 2        | 1.35          |
| (1,79)   | 1:A:77:VAL:HG21  | 1:A:68:MET:HE1  | 2        | 1.35          |
| (1,79)   | 1:A:77:VAL:HG21  | 1:A:68:MET:HE2  | 2        | 1.35          |
| (1,79)   | 1:A:77:VAL:HG21  | 1:A:68:MET:HE3  | 2        | 1.35          |
| (1,79)   | 1:A:77:VAL:HG22  | 1:A:68:MET:HE1  | 2        | 1.35          |
| (1,79)   | 1:A:77:VAL:HG22  | 1:A:68:MET:HE2  | 2        | 1.35          |
| (1,79)   | 1:A:77:VAL:HG22  | 1:A:68:MET:HE3  | 2        | 1.35          |
| (1,79)   | 1:A:77:VAL:HG23  | 1:A:68:MET:HE1  | 2        | 1.35          |
| (1,79)   | 1:A:77:VAL:HG23  | 1:A:68:MET:HE2  | 2        | 1.35          |
| (1,79)   | 1:A:77:VAL:HG23  | 1:A:68:MET:HE3  | 2        | 1.35          |
| (1,727)  | 1:A:133:ILE:HG21 | 1:A:145:VAL:HB  | 3        | 1.35          |
| (1,727)  | 1:A:133:ILE:HG22 | 1:A:145:VAL:HB  | 3        | 1.35          |
| (1,727)  | 1:A:133:ILE:HG23 | 1:A:145:VAL:HB  | 3        | 1.35          |
| (1,506)  | 1:A:114:ILE:HB   | 1:A:107:ARG:HD3 | 8        | 1.35          |
| (1,481)  | 1:A:113:PHE:HA   | 1:A:107:ARG:HB2 | 8        | 1.35          |
| (1,45)   | 1:A:75:PHE:HA    | 1:A:74:ARG:HG2  | 9        | 1.35          |
| (1,45)   | 1:A:75:PHE:HA    | 1:A:74:ARG:HG3  | 9        | 1.35          |
| (1,1754) | 1:A:118:PHE:HZ   | 1:B:116:ARG:HA  | 1        | 1.35          |
| (1,1594) | 1:B:133:ILE:HG21 | 1:B:145:VAL:HB  | 3        | 1.35          |
| (1,1594) | 1:B:133:ILE:HG22 | 1:B:145:VAL:HB  | 3        | 1.35          |
| (1,1594) | 1:B:133:ILE:HG23 | 1:B:145:VAL:HB  | 3        | 1.35          |
| (1,1373) | 1:B:114:ILE:HB   | 1:B:107:ARG:HD3 | 8        | 1.35          |
| (1,1058) | 1:B:84:PHE:HD1   | 1:B:82:LYS:H    | 4        | 1.35          |
| (1,1058) | 1:B:84:PHE:HD2   | 1:B:82:LYS:H    | 4        | 1.35          |
| (1,457)  | 1:A:111:HIS:H    | 1:A:109:ASP:HB2 | 6        | 1.34          |
| (1,457)  | 1:A:111:HIS:H    | 1:A:109:ASP:HB3 | 6        | 1.34          |
| (1,444)  | 1:A:108:GLN:HA   | 1:A:113:PHE:HE1 | 6        | 1.34          |
| (1,444)  | 1:A:108:GLN:HA   | 1:A:113:PHE:HE2 | 6        | 1.34          |
| (1,224)  | 1:A:87:GLU:H     | 1:A:88:GLU:HG2  | 5        | 1.34          |
| (1,224)  | 1:A:87:GLU:H     | 1:A:88:GLU:HG3  | 5        | 1.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,191)  | 1:A:84:PHE:HD1   | 1:A:82:LYS:H     | 4        | 1.34          |
| (1,191)  | 1:A:84:PHE:HD2   | 1:A:82:LYS:H     | 4        | 1.34          |
| (1,1745) | 1:A:114:ILE:H    | 1:B:121:LYS:H    | 6        | 1.34          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD11 | 5        | 1.34          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD12 | 5        | 1.34          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD13 | 5        | 1.34          |
| (1,1324) | 1:B:111:HIS:H    | 1:B:109:ASP:HB2  | 6        | 1.34          |
| (1,1324) | 1:B:111:HIS:H    | 1:B:109:ASP:HB3  | 6        | 1.34          |
| (1,1311) | 1:B:108:GLN:HA   | 1:B:113:PHE:HE1  | 6        | 1.34          |
| (1,1311) | 1:B:108:GLN:HA   | 1:B:113:PHE:HE2  | 6        | 1.34          |
| (1,1091) | 1:B:87:GLU:H     | 1:B:88:GLU:HG2   | 5        | 1.34          |
| (1,1091) | 1:B:87:GLU:H     | 1:B:88:GLU:HG3   | 5        | 1.34          |
| (1,887)  | 1:B:70:LEU:HB3   | 1:B:71:GLU:H     | 3        | 1.33          |
| (1,643)  | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD1  | 9        | 1.33          |
| (1,643)  | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD2  | 9        | 1.33          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD11 | 5        | 1.33          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD12 | 5        | 1.33          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD13 | 5        | 1.33          |
| (1,525)  | 1:A:115:SER:HB3  | 1:A:107:ARG:H    | 7        | 1.33          |
| (1,481)  | 1:A:113:PHE:HA   | 1:A:107:ARG:HB2  | 9        | 1.33          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD21  | 7        | 1.33          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD22  | 7        | 1.33          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD23  | 7        | 1.33          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD21  | 7        | 1.33          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD22  | 7        | 1.33          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD23  | 7        | 1.33          |
| (1,20)   | 1:A:70:LEU:HB3   | 1:A:71:GLU:H     | 3        | 1.33          |
| (1,190)  | 1:A:84:PHE:HE1   | 1:A:82:LYS:H     | 4        | 1.33          |
| (1,190)  | 1:A:84:PHE:HE2   | 1:A:82:LYS:H     | 4        | 1.33          |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD1  | 9        | 1.33          |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD2  | 9        | 1.33          |
| (1,1392) | 1:B:115:SER:HB3  | 1:B:107:ARG:H    | 7        | 1.33          |
| (1,1369) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HB2  | 5        | 1.33          |
| (1,1369) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HB2  | 5        | 1.33          |
| (1,1369) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HB2  | 5        | 1.33          |
| (1,1348) | 1:B:113:PHE:HA   | 1:B:107:ARG:HB2  | 9        | 1.33          |
| (1,1288) | 1:B:107:ARG:HD2  | 1:B:105:GLU:H    | 5        | 1.33          |
| (1,1209) | 1:B:98:ILE:HD11  | 1:B:122:TYR:HD1  | 8        | 1.33          |
| (1,1209) | 1:B:98:ILE:HD11  | 1:B:122:TYR:HD2  | 8        | 1.33          |
| (1,1209) | 1:B:98:ILE:HD12  | 1:B:122:TYR:HD1  | 8        | 1.33          |
| (1,1209) | 1:B:98:ILE:HD12  | 1:B:122:TYR:HD2  | 8        | 1.33          |
| (1,1209) | 1:B:98:ILE:HD13  | 1:B:122:TYR:HD1  | 8        | 1.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1209) | 1:B:98:ILE:HD13  | 1:B:122:TYR:HD2  | 8        | 1.33          |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD21  | 7        | 1.33          |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD22  | 7        | 1.33          |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD23  | 7        | 1.33          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD21  | 7        | 1.33          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD22  | 7        | 1.33          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD23  | 7        | 1.33          |
| (1,1057) | 1:B:84:PHE:HE1   | 1:B:82:LYS:H     | 4        | 1.33          |
| (1,1057) | 1:B:84:PHE:HE2   | 1:B:82:LYS:H     | 4        | 1.33          |
| (1,99)   | 1:A:77:VAL:HG21  | 1:A:78:ASN:HB2   | 5        | 1.32          |
| (1,99)   | 1:A:77:VAL:HG22  | 1:A:78:ASN:HB2   | 5        | 1.32          |
| (1,99)   | 1:A:77:VAL:HG23  | 1:A:78:ASN:HB2   | 5        | 1.32          |
| (1,966)  | 1:B:77:VAL:HG21  | 1:B:78:ASN:HB2   | 5        | 1.32          |
| (1,966)  | 1:B:77:VAL:HG22  | 1:B:78:ASN:HB2   | 5        | 1.32          |
| (1,966)  | 1:B:77:VAL:HG23  | 1:B:78:ASN:HB2   | 5        | 1.32          |
| (1,887)  | 1:B:70:LEU:HB3   | 1:B:71:GLU:H     | 1        | 1.32          |
| (1,887)  | 1:B:70:LEU:HB3   | 1:B:71:GLU:H     | 5        | 1.32          |
| (1,502)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HB2  | 5        | 1.32          |
| (1,502)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HB2  | 5        | 1.32          |
| (1,502)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HB2  | 5        | 1.32          |
| (1,421)  | 1:A:107:ARG:HD2  | 1:A:105:GLU:H    | 5        | 1.32          |
| (1,342)  | 1:A:98:ILE:HD11  | 1:A:122:TYR:HD1  | 8        | 1.32          |
| (1,342)  | 1:A:98:ILE:HD11  | 1:A:122:TYR:HD2  | 8        | 1.32          |
| (1,342)  | 1:A:98:ILE:HD12  | 1:A:122:TYR:HD1  | 8        | 1.32          |
| (1,342)  | 1:A:98:ILE:HD12  | 1:A:122:TYR:HD2  | 8        | 1.32          |
| (1,342)  | 1:A:98:ILE:HD13  | 1:A:122:TYR:HD1  | 8        | 1.32          |
| (1,342)  | 1:A:98:ILE:HD13  | 1:A:122:TYR:HD2  | 8        | 1.32          |
| (1,20)   | 1:A:70:LEU:HB3   | 1:A:71:GLU:H     | 1        | 1.32          |
| (1,20)   | 1:A:70:LEU:HB3   | 1:A:71:GLU:H     | 5        | 1.32          |
| (1,890)  | 1:B:70:LEU:HB2   | 1:B:74:ARG:H     | 6        | 1.31          |
| (1,887)  | 1:B:70:LEU:HB3   | 1:B:71:GLU:H     | 4        | 1.31          |
| (1,618)  | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD1  | 7        | 1.31          |
| (1,618)  | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD2  | 7        | 1.31          |
| (1,618)  | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD1  | 7        | 1.31          |
| (1,618)  | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD2  | 7        | 1.31          |
| (1,618)  | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD1  | 7        | 1.31          |
| (1,618)  | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD2  | 7        | 1.31          |
| (1,516)  | 1:A:114:ILE:H    | 1:A:114:ILE:HG12 | 2        | 1.31          |
| (1,23)   | 1:A:70:LEU:HB2   | 1:A:74:ARG:H     | 6        | 1.31          |
| (1,20)   | 1:A:70:LEU:HB3   | 1:A:71:GLU:H     | 4        | 1.31          |
| (1,184)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 5        | 1.31          |
| (1,183)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 5        | 1.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD1  | 7        | 1.31          |
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD2  | 7        | 1.31          |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD1  | 7        | 1.31          |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD2  | 7        | 1.31          |
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD1  | 7        | 1.31          |
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD2  | 7        | 1.31          |
| (1,1383) | 1:B:114:ILE:H    | 1:B:114:ILE:HG12 | 2        | 1.31          |
| (1,1051) | 1:B:83:HIS:H     | 1:B:84:PHE:H     | 5        | 1.31          |
| (1,1050) | 1:B:83:HIS:H     | 1:B:84:PHE:H     | 5        | 1.31          |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB2  | 4        | 1.3           |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB3  | 4        | 1.3           |
| (1,520)  | 1:A:115:SER:HA   | 1:A:104:HIS:HE1  | 7        | 1.3           |
| (1,435)  | 1:A:107:ARG:HB3  | 1:A:109:ASP:H    | 3        | 1.3           |
| (1,188)  | 1:A:83:HIS:H     | 1:A:141:GLY:HA2  | 9        | 1.3           |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB2  | 4        | 1.3           |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB3  | 4        | 1.3           |
| (1,1387) | 1:B:115:SER:HA   | 1:B:104:HIS:HE1  | 7        | 1.3           |
| (1,1302) | 1:B:107:ARG:HB3  | 1:B:109:ASP:H    | 3        | 1.3           |
| (1,1055) | 1:B:83:HIS:H     | 1:B:141:GLY:HA2  | 9        | 1.3           |
| (1,516)  | 1:A:114:ILE:H    | 1:A:114:ILE:HG12 | 7        | 1.29          |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG21 | 9        | 1.29          |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG22 | 9        | 1.29          |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG23 | 9        | 1.29          |
| (1,258)  | 1:A:89:LEU:HD11  | 1:A:102:GLY:HA2  | 6        | 1.29          |
| (1,258)  | 1:A:89:LEU:HD12  | 1:A:102:GLY:HA2  | 6        | 1.29          |
| (1,258)  | 1:A:89:LEU:HD13  | 1:A:102:GLY:HA2  | 6        | 1.29          |
| (1,257)  | 1:A:89:LEU:HD11  | 1:A:102:GLY:HA2  | 6        | 1.29          |
| (1,257)  | 1:A:89:LEU:HD12  | 1:A:102:GLY:HA2  | 6        | 1.29          |
| (1,257)  | 1:A:89:LEU:HD13  | 1:A:102:GLY:HA2  | 6        | 1.29          |
| (1,170)  | 1:A:83:HIS:H     | 1:A:81:VAL:HB    | 7        | 1.29          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG21 | 9        | 1.29          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG22 | 9        | 1.29          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG23 | 9        | 1.29          |
| (1,1125) | 1:B:89:LEU:HD11  | 1:B:102:GLY:HA2  | 6        | 1.29          |
| (1,1125) | 1:B:89:LEU:HD12  | 1:B:102:GLY:HA2  | 6        | 1.29          |
| (1,1125) | 1:B:89:LEU:HD13  | 1:B:102:GLY:HA2  | 6        | 1.29          |
| (1,1124) | 1:B:89:LEU:HD11  | 1:B:102:GLY:HA2  | 6        | 1.29          |
| (1,1124) | 1:B:89:LEU:HD12  | 1:B:102:GLY:HA2  | 6        | 1.29          |
| (1,1124) | 1:B:89:LEU:HD13  | 1:B:102:GLY:HA2  | 6        | 1.29          |
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB2   | 1        | 1.29          |
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB3   | 1        | 1.29          |
| (1,1037) | 1:B:83:HIS:H     | 1:B:81:VAL:HB    | 7        | 1.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,953)  | 1:B:77:VAL:HG21  | 1:B:75:PHE:HZ    | 1        | 1.28          |
| (1,953)  | 1:B:77:VAL:HG22  | 1:B:75:PHE:HZ    | 1        | 1.28          |
| (1,953)  | 1:B:77:VAL:HG23  | 1:B:75:PHE:HZ    | 1        | 1.28          |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE1   | 3        | 1.28          |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE2   | 3        | 1.28          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE1   | 3        | 1.28          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE2   | 3        | 1.28          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE1   | 3        | 1.28          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE2   | 3        | 1.28          |
| (1,506)  | 1:A:114:ILE:HB   | 1:A:107:ARG:HD3  | 6        | 1.28          |
| (1,258)  | 1:A:89:LEU:HD11  | 1:A:102:GLY:HA2  | 8        | 1.28          |
| (1,258)  | 1:A:89:LEU:HD12  | 1:A:102:GLY:HA2  | 8        | 1.28          |
| (1,258)  | 1:A:89:LEU:HD13  | 1:A:102:GLY:HA2  | 8        | 1.28          |
| (1,257)  | 1:A:89:LEU:HD11  | 1:A:102:GLY:HA2  | 8        | 1.28          |
| (1,257)  | 1:A:89:LEU:HD12  | 1:A:102:GLY:HA2  | 8        | 1.28          |
| (1,257)  | 1:A:89:LEU:HD13  | 1:A:102:GLY:HA2  | 8        | 1.28          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB2   | 1        | 1.28          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB3   | 1        | 1.28          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE1   | 3        | 1.28          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE2   | 3        | 1.28          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE1   | 3        | 1.28          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE2   | 3        | 1.28          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE1   | 3        | 1.28          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE2   | 3        | 1.28          |
| (1,1383) | 1:B:114:ILE:H    | 1:B:114:ILE:HG12 | 7        | 1.28          |
| (1,1373) | 1:B:114:ILE:HB   | 1:B:107:ARG:HD3  | 6        | 1.28          |
| (1,1125) | 1:B:89:LEU:HD11  | 1:B:102:GLY:HA2  | 8        | 1.28          |
| (1,1125) | 1:B:89:LEU:HD12  | 1:B:102:GLY:HA2  | 8        | 1.28          |
| (1,1125) | 1:B:89:LEU:HD13  | 1:B:102:GLY:HA2  | 8        | 1.28          |
| (1,1124) | 1:B:89:LEU:HD11  | 1:B:102:GLY:HA2  | 8        | 1.28          |
| (1,1124) | 1:B:89:LEU:HD12  | 1:B:102:GLY:HA2  | 8        | 1.28          |
| (1,1124) | 1:B:89:LEU:HD13  | 1:B:102:GLY:HA2  | 8        | 1.28          |
| (1,887)  | 1:B:70:LEU:HB3   | 1:B:71:GLU:H     | 9        | 1.27          |
| (1,550)  | 1:A:118:PHE:HE1  | 1:A:102:GLY:H    | 6        | 1.27          |
| (1,550)  | 1:A:118:PHE:HE2  | 1:A:102:GLY:H    | 6        | 1.27          |
| (1,509)  | 1:A:114:ILE:HG21 | 1:A:109:ASP:H    | 4        | 1.27          |
| (1,509)  | 1:A:114:ILE:HG22 | 1:A:109:ASP:H    | 4        | 1.27          |
| (1,509)  | 1:A:114:ILE:HG23 | 1:A:109:ASP:H    | 4        | 1.27          |
| (1,20)   | 1:A:70:LEU:HB3   | 1:A:71:GLU:H     | 9        | 1.27          |
| (1,1417) | 1:B:118:PHE:HE1  | 1:B:102:GLY:H    | 6        | 1.27          |
| (1,1417) | 1:B:118:PHE:HE2  | 1:B:102:GLY:H    | 6        | 1.27          |
| (1,1376) | 1:B:114:ILE:HG21 | 1:B:109:ASP:H    | 4        | 1.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1376) | 1:B:114:ILE:HG22 | 1:B:109:ASP:H    | 4        | 1.27          |
| (1,1376) | 1:B:114:ILE:HG23 | 1:B:109:ASP:H    | 4        | 1.27          |
| (1,1311) | 1:B:108:GLN:HA   | 1:B:113:PHE:HE1  | 8        | 1.27          |
| (1,1311) | 1:B:108:GLN:HA   | 1:B:113:PHE:HE2  | 8        | 1.27          |
| (1,954)  | 1:B:77:VAL:HG21  | 1:B:75:PHE:HD1   | 9        | 1.26          |
| (1,954)  | 1:B:77:VAL:HG21  | 1:B:75:PHE:HD2   | 9        | 1.26          |
| (1,954)  | 1:B:77:VAL:HG22  | 1:B:75:PHE:HD1   | 9        | 1.26          |
| (1,954)  | 1:B:77:VAL:HG22  | 1:B:75:PHE:HD2   | 9        | 1.26          |
| (1,954)  | 1:B:77:VAL:HG23  | 1:B:75:PHE:HD1   | 9        | 1.26          |
| (1,954)  | 1:B:77:VAL:HG23  | 1:B:75:PHE:HD2   | 9        | 1.26          |
| (1,87)   | 1:A:77:VAL:HG21  | 1:A:75:PHE:HD1   | 9        | 1.26          |
| (1,87)   | 1:A:77:VAL:HG21  | 1:A:75:PHE:HD2   | 9        | 1.26          |
| (1,87)   | 1:A:77:VAL:HG22  | 1:A:75:PHE:HD1   | 9        | 1.26          |
| (1,87)   | 1:A:77:VAL:HG22  | 1:A:75:PHE:HD2   | 9        | 1.26          |
| (1,87)   | 1:A:77:VAL:HG23  | 1:A:75:PHE:HD1   | 9        | 1.26          |
| (1,87)   | 1:A:77:VAL:HG23  | 1:A:75:PHE:HD2   | 9        | 1.26          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG21 | 8        | 1.26          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG22 | 8        | 1.26          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG23 | 8        | 1.26          |
| (1,564)  | 1:A:118:PHE:HD1  | 1:A:118:PHE:H    | 2        | 1.26          |
| (1,564)  | 1:A:118:PHE:HD2  | 1:A:118:PHE:H    | 2        | 1.26          |
| (1,444)  | 1:A:108:GLN:HA   | 1:A:113:PHE:HE1  | 8        | 1.26          |
| (1,444)  | 1:A:108:GLN:HA   | 1:A:113:PHE:HE2  | 8        | 1.26          |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG21 | 1        | 1.26          |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG22 | 1        | 1.26          |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG23 | 1        | 1.26          |
| (1,435)  | 1:A:107:ARG:HB3  | 1:A:109:ASP:H    | 4        | 1.26          |
| (1,166)  | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD1  | 7        | 1.26          |
| (1,166)  | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD2  | 7        | 1.26          |
| (1,166)  | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD1  | 7        | 1.26          |
| (1,166)  | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD2  | 7        | 1.26          |
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD1  | 7        | 1.26          |
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD2  | 7        | 1.26          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG21 | 8        | 1.26          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG22 | 8        | 1.26          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG23 | 8        | 1.26          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG21 | 1        | 1.26          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG22 | 1        | 1.26          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG23 | 1        | 1.26          |
| (1,1302) | 1:B:107:ARG:HB3  | 1:B:109:ASP:H    | 4        | 1.26          |
| (1,1033) | 1:B:81:VAL:HG11  | 1:B:118:PHE:HD1  | 7        | 1.26          |
| (1,1033) | 1:B:81:VAL:HG11  | 1:B:118:PHE:HD2  | 7        | 1.26          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1033) | 1:B:81:VAL:HG12  | 1:B:118:PHE:HD1 | 7        | 1.26          |
| (1,1033) | 1:B:81:VAL:HG12  | 1:B:118:PHE:HD2 | 7        | 1.26          |
| (1,1033) | 1:B:81:VAL:HG13  | 1:B:118:PHE:HD1 | 7        | 1.26          |
| (1,1033) | 1:B:81:VAL:HG13  | 1:B:118:PHE:HD2 | 7        | 1.26          |
| (1,949)  | 1:B:77:VAL:HG21  | 1:B:68:MET:HA   | 2        | 1.25          |
| (1,949)  | 1:B:77:VAL:HG22  | 1:B:68:MET:HA   | 2        | 1.25          |
| (1,949)  | 1:B:77:VAL:HG23  | 1:B:68:MET:HA   | 2        | 1.25          |
| (1,82)   | 1:A:77:VAL:HG21  | 1:A:68:MET:HA   | 2        | 1.25          |
| (1,82)   | 1:A:77:VAL:HG22  | 1:A:68:MET:HA   | 2        | 1.25          |
| (1,82)   | 1:A:77:VAL:HG23  | 1:A:68:MET:HA   | 2        | 1.25          |
| (1,501)  | 1:A:114:ILE:HD11 | 1:A:104:HIS:HE1 | 8        | 1.25          |
| (1,501)  | 1:A:114:ILE:HD12 | 1:A:104:HIS:HE1 | 8        | 1.25          |
| (1,501)  | 1:A:114:ILE:HD13 | 1:A:104:HIS:HE1 | 8        | 1.25          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB2  | 1        | 1.25          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB3  | 1        | 1.25          |
| (1,150)  | 1:A:81:VAL:HG11  | 1:A:79:LEU:HB2  | 4        | 1.25          |
| (1,150)  | 1:A:81:VAL:HG11  | 1:A:79:LEU:HB3  | 4        | 1.25          |
| (1,150)  | 1:A:81:VAL:HG12  | 1:A:79:LEU:HB2  | 4        | 1.25          |
| (1,150)  | 1:A:81:VAL:HG12  | 1:A:79:LEU:HB3  | 4        | 1.25          |
| (1,150)  | 1:A:81:VAL:HG13  | 1:A:79:LEU:HB2  | 4        | 1.25          |
| (1,150)  | 1:A:81:VAL:HG13  | 1:A:79:LEU:HB3  | 4        | 1.25          |
| (1,1431) | 1:B:118:PHE:HD1  | 1:B:118:PHE:H   | 2        | 1.25          |
| (1,1431) | 1:B:118:PHE:HD2  | 1:B:118:PHE:H   | 2        | 1.25          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB2  | 1        | 1.25          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB3  | 1        | 1.25          |
| (1,1017) | 1:B:81:VAL:HG11  | 1:B:79:LEU:HB2  | 4        | 1.25          |
| (1,1017) | 1:B:81:VAL:HG11  | 1:B:79:LEU:HB3  | 4        | 1.25          |
| (1,1017) | 1:B:81:VAL:HG12  | 1:B:79:LEU:HB2  | 4        | 1.25          |
| (1,1017) | 1:B:81:VAL:HG12  | 1:B:79:LEU:HB3  | 4        | 1.25          |
| (1,1017) | 1:B:81:VAL:HG13  | 1:B:79:LEU:HB2  | 4        | 1.25          |
| (1,1017) | 1:B:81:VAL:HG13  | 1:B:79:LEU:HB3  | 4        | 1.25          |
| (1,993)  | 1:B:78:ASN:H     | 1:B:78:ASN:HD22 | 9        | 1.24          |
| (1,99)   | 1:A:77:VAL:HG21  | 1:A:78:ASN:HB2  | 3        | 1.24          |
| (1,99)   | 1:A:77:VAL:HG22  | 1:A:78:ASN:HB2  | 3        | 1.24          |
| (1,99)   | 1:A:77:VAL:HG23  | 1:A:78:ASN:HB2  | 3        | 1.24          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB2  | 3        | 1.24          |
| (1,298)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HB3  | 3        | 1.24          |
| (1,254)  | 1:A:89:LEU:HD11  | 1:A:91:VAL:HB   | 4        | 1.24          |
| (1,254)  | 1:A:89:LEU:HD12  | 1:A:91:VAL:HB   | 4        | 1.24          |
| (1,254)  | 1:A:89:LEU:HD13  | 1:A:91:VAL:HB   | 4        | 1.24          |
| (1,195)  | 1:A:84:PHE:HD1   | 1:A:84:PHE:H    | 9        | 1.24          |
| (1,195)  | 1:A:84:PHE:HD2   | 1:A:84:PHE:H    | 9        | 1.24          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,194)  | 1:A:84:PHE:HD1   | 1:A:83:HIS:H    | 9        | 1.24          |
| (1,194)  | 1:A:84:PHE:HD2   | 1:A:83:HIS:H    | 9        | 1.24          |
| (1,1368) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HE1 | 8        | 1.24          |
| (1,1368) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HE1 | 8        | 1.24          |
| (1,1368) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HE1 | 8        | 1.24          |
| (1,126)  | 1:A:78:ASN:H     | 1:A:78:ASN:HD22 | 9        | 1.24          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB2  | 3        | 1.24          |
| (1,1165) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HB3  | 3        | 1.24          |
| (1,1121) | 1:B:89:LEU:HD11  | 1:B:91:VAL:HB   | 4        | 1.24          |
| (1,1121) | 1:B:89:LEU:HD12  | 1:B:91:VAL:HB   | 4        | 1.24          |
| (1,1121) | 1:B:89:LEU:HD13  | 1:B:91:VAL:HB   | 4        | 1.24          |
| (1,1062) | 1:B:84:PHE:HD1   | 1:B:84:PHE:H    | 9        | 1.24          |
| (1,1062) | 1:B:84:PHE:HD2   | 1:B:84:PHE:H    | 9        | 1.24          |
| (1,1061) | 1:B:84:PHE:HD1   | 1:B:83:HIS:H    | 9        | 1.24          |
| (1,1061) | 1:B:84:PHE:HD2   | 1:B:83:HIS:H    | 9        | 1.24          |
| (1,99)   | 1:A:77:VAL:HG21  | 1:A:78:ASN:HB2  | 4        | 1.23          |
| (1,99)   | 1:A:77:VAL:HG22  | 1:A:78:ASN:HB2  | 4        | 1.23          |
| (1,99)   | 1:A:77:VAL:HG23  | 1:A:78:ASN:HB2  | 4        | 1.23          |
| (1,99)   | 1:A:77:VAL:HG21  | 1:A:78:ASN:HB2  | 8        | 1.23          |
| (1,99)   | 1:A:77:VAL:HG22  | 1:A:78:ASN:HB2  | 8        | 1.23          |
| (1,99)   | 1:A:77:VAL:HG23  | 1:A:78:ASN:HB2  | 8        | 1.23          |
| (1,966)  | 1:B:77:VAL:HG21  | 1:B:78:ASN:HB2  | 3        | 1.23          |
| (1,966)  | 1:B:77:VAL:HG22  | 1:B:78:ASN:HB2  | 3        | 1.23          |
| (1,966)  | 1:B:77:VAL:HG23  | 1:B:78:ASN:HB2  | 3        | 1.23          |
| (1,966)  | 1:B:77:VAL:HG21  | 1:B:78:ASN:HB2  | 4        | 1.23          |
| (1,966)  | 1:B:77:VAL:HG22  | 1:B:78:ASN:HB2  | 4        | 1.23          |
| (1,966)  | 1:B:77:VAL:HG23  | 1:B:78:ASN:HB2  | 4        | 1.23          |
| (1,966)  | 1:B:77:VAL:HG21  | 1:B:78:ASN:HB2  | 8        | 1.23          |
| (1,966)  | 1:B:77:VAL:HG22  | 1:B:78:ASN:HB2  | 8        | 1.23          |
| (1,966)  | 1:B:77:VAL:HG23  | 1:B:78:ASN:HB2  | 8        | 1.23          |
| (1,818)  | 1:A:145:VAL:HG11 | 1:A:145:VAL:H   | 3        | 1.23          |
| (1,818)  | 1:A:145:VAL:HG12 | 1:A:145:VAL:H   | 3        | 1.23          |
| (1,818)  | 1:A:145:VAL:HG13 | 1:A:145:VAL:H   | 3        | 1.23          |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB2 | 5        | 1.23          |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB3 | 5        | 1.23          |
| (1,236)  | 1:A:89:LEU:HD21  | 1:A:85:SER:HB3  | 6        | 1.23          |
| (1,236)  | 1:A:89:LEU:HD22  | 1:A:85:SER:HB3  | 6        | 1.23          |
| (1,236)  | 1:A:89:LEU:HD23  | 1:A:85:SER:HB3  | 6        | 1.23          |
| (1,1685) | 1:B:145:VAL:HG11 | 1:B:145:VAL:H   | 3        | 1.23          |
| (1,1685) | 1:B:145:VAL:HG12 | 1:B:145:VAL:H   | 3        | 1.23          |
| (1,1685) | 1:B:145:VAL:HG13 | 1:B:145:VAL:H   | 3        | 1.23          |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB2 | 5        | 1.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB3  | 5        | 1.23          |
| (1,1103) | 1:B:89:LEU:HD21  | 1:B:85:SER:HB3   | 6        | 1.23          |
| (1,1103) | 1:B:89:LEU:HD22  | 1:B:85:SER:HB3   | 6        | 1.23          |
| (1,1103) | 1:B:89:LEU:HD23  | 1:B:85:SER:HB3   | 6        | 1.23          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD1   | 1        | 1.23          |
| (1,1084) | 1:B:86:PRO:HB2   | 1:B:84:PHE:HD2   | 1        | 1.23          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD1   | 1        | 1.23          |
| (1,1084) | 1:B:86:PRO:HB3   | 1:B:84:PHE:HD2   | 1        | 1.23          |
| (1,985)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB2  | 6        | 1.22          |
| (1,98)   | 1:A:77:VAL:HG11  | 1:A:77:VAL:H     | 9        | 1.22          |
| (1,98)   | 1:A:77:VAL:HG12  | 1:A:77:VAL:H     | 9        | 1.22          |
| (1,98)   | 1:A:77:VAL:HG13  | 1:A:77:VAL:H     | 9        | 1.22          |
| (1,965)  | 1:B:77:VAL:HG11  | 1:B:77:VAL:H     | 9        | 1.22          |
| (1,965)  | 1:B:77:VAL:HG12  | 1:B:77:VAL:H     | 9        | 1.22          |
| (1,965)  | 1:B:77:VAL:HG13  | 1:B:77:VAL:H     | 9        | 1.22          |
| (1,954)  | 1:B:77:VAL:HG21  | 1:B:75:PHE:HD1   | 8        | 1.22          |
| (1,954)  | 1:B:77:VAL:HG21  | 1:B:75:PHE:HD2   | 8        | 1.22          |
| (1,954)  | 1:B:77:VAL:HG22  | 1:B:75:PHE:HD1   | 8        | 1.22          |
| (1,954)  | 1:B:77:VAL:HG22  | 1:B:75:PHE:HD2   | 8        | 1.22          |
| (1,954)  | 1:B:77:VAL:HG23  | 1:B:75:PHE:HD1   | 8        | 1.22          |
| (1,954)  | 1:B:77:VAL:HG23  | 1:B:75:PHE:HD2   | 8        | 1.22          |
| (1,87)   | 1:A:77:VAL:HG21  | 1:A:75:PHE:HD1   | 8        | 1.22          |
| (1,87)   | 1:A:77:VAL:HG21  | 1:A:75:PHE:HD2   | 8        | 1.22          |
| (1,87)   | 1:A:77:VAL:HG22  | 1:A:75:PHE:HD1   | 8        | 1.22          |
| (1,87)   | 1:A:77:VAL:HG22  | 1:A:75:PHE:HD2   | 8        | 1.22          |
| (1,87)   | 1:A:77:VAL:HG23  | 1:A:75:PHE:HD1   | 8        | 1.22          |
| (1,87)   | 1:A:77:VAL:HG23  | 1:A:75:PHE:HD2   | 8        | 1.22          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD1   | 1        | 1.22          |
| (1,217)  | 1:A:86:PRO:HB2   | 1:A:84:PHE:HD2   | 1        | 1.22          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD1   | 1        | 1.22          |
| (1,217)  | 1:A:86:PRO:HB3   | 1:A:84:PHE:HD2   | 1        | 1.22          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG12 | 2        | 1.22          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG13 | 2        | 1.22          |
| (1,118)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB2  | 6        | 1.22          |
| (1,993)  | 1:B:78:ASN:H     | 1:B:78:ASN:HD22  | 2        | 1.21          |
| (1,639)  | 1:A:124:ILE:HD11 | 1:A:128:VAL:H    | 4        | 1.21          |
| (1,639)  | 1:A:124:ILE:HD12 | 1:A:128:VAL:H    | 4        | 1.21          |
| (1,639)  | 1:A:124:ILE:HD13 | 1:A:128:VAL:H    | 4        | 1.21          |
| (1,595)  | 1:A:122:TYR:HD1  | 1:A:122:TYR:H    | 9        | 1.21          |
| (1,595)  | 1:A:122:TYR:HD2  | 1:A:122:TYR:H    | 9        | 1.21          |
| (1,551)  | 1:A:118:PHE:HD1  | 1:A:103:LYS:HA   | 6        | 1.21          |
| (1,551)  | 1:A:118:PHE:HD2  | 1:A:103:LYS:HA   | 6        | 1.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,421)  | 1:A:107:ARG:HD2  | 1:A:105:GLU:H    | 6        | 1.21          |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG2   | 7        | 1.21          |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG3   | 7        | 1.21          |
| (1,1462) | 1:B:122:TYR:HD1  | 1:B:122:TYR:H    | 9        | 1.21          |
| (1,1462) | 1:B:122:TYR:HD2  | 1:B:122:TYR:H    | 9        | 1.21          |
| (1,1418) | 1:B:118:PHE:HD1  | 1:B:103:LYS:HA   | 6        | 1.21          |
| (1,1418) | 1:B:118:PHE:HD2  | 1:B:103:LYS:HA   | 6        | 1.21          |
| (1,1288) | 1:B:107:ARG:HD2  | 1:B:105:GLU:H    | 6        | 1.21          |
| (1,126)  | 1:A:78:ASN:H     | 1:A:78:ASN:HD22  | 2        | 1.21          |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG2   | 7        | 1.21          |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG3   | 7        | 1.21          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD11  | 6        | 1.2           |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD12  | 6        | 1.2           |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD13  | 6        | 1.2           |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD11  | 6        | 1.2           |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD12  | 6        | 1.2           |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD13  | 6        | 1.2           |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD11  | 6        | 1.2           |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD12  | 6        | 1.2           |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD13  | 6        | 1.2           |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD11  | 6        | 1.2           |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD12  | 6        | 1.2           |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD13  | 6        | 1.2           |
| (1,507)  | 1:A:114:ILE:HD11 | 1:A:107:ARG:HD3  | 9        | 1.2           |
| (1,507)  | 1:A:114:ILE:HD12 | 1:A:107:ARG:HD3  | 9        | 1.2           |
| (1,507)  | 1:A:114:ILE:HD13 | 1:A:107:ARG:HD3  | 9        | 1.2           |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG21 | 2        | 1.2           |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG22 | 2        | 1.2           |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG23 | 2        | 1.2           |
| (1,170)  | 1:A:83:HIS:H     | 1:A:81:VAL:HB    | 1        | 1.2           |
| (1,1506) | 1:B:124:ILE:HD11 | 1:B:128:VAL:H    | 4        | 1.2           |
| (1,1506) | 1:B:124:ILE:HD12 | 1:B:128:VAL:H    | 4        | 1.2           |
| (1,1506) | 1:B:124:ILE:HD13 | 1:B:128:VAL:H    | 4        | 1.2           |
| (1,1374) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HD3  | 9        | 1.2           |
| (1,1374) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HD3  | 9        | 1.2           |
| (1,1374) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HD3  | 9        | 1.2           |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG21 | 2        | 1.2           |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG22 | 2        | 1.2           |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG23 | 2        | 1.2           |
| (1,1121) | 1:B:89:LEU:HD11  | 1:B:91:VAL:HB    | 9        | 1.2           |
| (1,1121) | 1:B:89:LEU:HD12  | 1:B:91:VAL:HB    | 9        | 1.2           |
| (1,1121) | 1:B:89:LEU:HD13  | 1:B:91:VAL:HB    | 9        | 1.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1090) | 1:B:87:GLU:H    | 1:B:88:GLU:HB2   | 2        | 1.2           |
| (1,1090) | 1:B:87:GLU:H    | 1:B:88:GLU:HB3   | 2        | 1.2           |
| (1,1037) | 1:B:83:HIS:H    | 1:B:81:VAL:HB    | 1        | 1.2           |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG21 | 3        | 1.19          |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG22 | 3        | 1.19          |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG23 | 3        | 1.19          |
| (1,568)  | 1:A:119:HIS:HB3 | 1:A:101:HIS:HA   | 3        | 1.19          |
| (1,564)  | 1:A:118:PHE:HD1 | 1:A:118:PHE:H    | 6        | 1.19          |
| (1,564)  | 1:A:118:PHE:HD2 | 1:A:118:PHE:H    | 6        | 1.19          |
| (1,516)  | 1:A:114:ILE:H   | 1:A:114:ILE:HG12 | 9        | 1.19          |
| (1,342)  | 1:A:98:ILE:HD11 | 1:A:122:TYR:HD1  | 3        | 1.19          |
| (1,342)  | 1:A:98:ILE:HD11 | 1:A:122:TYR:HD2  | 3        | 1.19          |
| (1,342)  | 1:A:98:ILE:HD12 | 1:A:122:TYR:HD1  | 3        | 1.19          |
| (1,342)  | 1:A:98:ILE:HD12 | 1:A:122:TYR:HD2  | 3        | 1.19          |
| (1,342)  | 1:A:98:ILE:HD13 | 1:A:122:TYR:HD1  | 3        | 1.19          |
| (1,342)  | 1:A:98:ILE:HD13 | 1:A:122:TYR:HD2  | 3        | 1.19          |
| (1,267)  | 1:A:90:LYS:HB2  | 1:A:101:HIS:HB3  | 2        | 1.19          |
| (1,267)  | 1:A:90:LYS:HB3  | 1:A:101:HIS:HB3  | 2        | 1.19          |
| (1,254)  | 1:A:89:LEU:HD11 | 1:A:91:VAL:HB    | 9        | 1.19          |
| (1,254)  | 1:A:89:LEU:HD12 | 1:A:91:VAL:HB    | 9        | 1.19          |
| (1,254)  | 1:A:89:LEU:HD13 | 1:A:91:VAL:HB    | 9        | 1.19          |
| (1,223)  | 1:A:87:GLU:H    | 1:A:88:GLU:HB2   | 2        | 1.19          |
| (1,223)  | 1:A:87:GLU:H    | 1:A:88:GLU:HB3   | 2        | 1.19          |
| (1,190)  | 1:A:84:PHE:HE1  | 1:A:82:LYS:H     | 8        | 1.19          |
| (1,190)  | 1:A:84:PHE:HE2  | 1:A:82:LYS:H     | 8        | 1.19          |
| (1,1745) | 1:A:114:ILE:H   | 1:B:121:LYS:H    | 4        | 1.19          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG21 | 3        | 1.19          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG22 | 3        | 1.19          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG23 | 3        | 1.19          |
| (1,1435) | 1:B:119:HIS:HB3 | 1:B:101:HIS:HA   | 3        | 1.19          |
| (1,1383) | 1:B:114:ILE:H   | 1:B:114:ILE:HG12 | 9        | 1.19          |
| (1,1209) | 1:B:98:ILE:HD11 | 1:B:122:TYR:HD1  | 3        | 1.19          |
| (1,1209) | 1:B:98:ILE:HD11 | 1:B:122:TYR:HD2  | 3        | 1.19          |
| (1,1209) | 1:B:98:ILE:HD12 | 1:B:122:TYR:HD1  | 3        | 1.19          |
| (1,1209) | 1:B:98:ILE:HD12 | 1:B:122:TYR:HD2  | 3        | 1.19          |
| (1,1209) | 1:B:98:ILE:HD13 | 1:B:122:TYR:HD1  | 3        | 1.19          |
| (1,1209) | 1:B:98:ILE:HD13 | 1:B:122:TYR:HD2  | 3        | 1.19          |
| (1,1134) | 1:B:90:LYS:HB2  | 1:B:101:HIS:HB3  | 2        | 1.19          |
| (1,1134) | 1:B:90:LYS:HB3  | 1:B:101:HIS:HB3  | 2        | 1.19          |
| (1,976)  | 1:B:77:VAL:HG21 | 1:B:79:LEU:H     | 3        | 1.18          |
| (1,976)  | 1:B:77:VAL:HG22 | 1:B:79:LEU:H     | 3        | 1.18          |
| (1,976)  | 1:B:77:VAL:HG23 | 1:B:79:LEU:H     | 3        | 1.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,813)  | 1:A:145:VAL:HA   | 1:A:135:SER:H    | 1        | 1.18          |
| (1,734)  | 1:A:135:SER:H    | 1:A:134:THR:HB   | 2        | 1.18          |
| (1,444)  | 1:A:108:GLN:HA   | 1:A:113:PHE:HE1  | 5        | 1.18          |
| (1,444)  | 1:A:108:GLN:HA   | 1:A:113:PHE:HE2  | 5        | 1.18          |
| (1,365)  | 1:A:100:VAL:HG11 | 1:A:102:GLY:H    | 5        | 1.18          |
| (1,365)  | 1:A:100:VAL:HG12 | 1:A:102:GLY:H    | 5        | 1.18          |
| (1,365)  | 1:A:100:VAL:HG13 | 1:A:102:GLY:H    | 5        | 1.18          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG12 | 5        | 1.18          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG13 | 5        | 1.18          |
| (1,1680) | 1:B:145:VAL:HA   | 1:B:135:SER:H    | 1        | 1.18          |
| (1,1601) | 1:B:135:SER:H    | 1:B:134:THR:HB   | 2        | 1.18          |
| (1,1591) | 1:B:133:ILE:HD11 | 1:B:134:THR:H    | 5        | 1.18          |
| (1,1591) | 1:B:133:ILE:HD12 | 1:B:134:THR:H    | 5        | 1.18          |
| (1,1591) | 1:B:133:ILE:HD13 | 1:B:134:THR:H    | 5        | 1.18          |
| (1,150)  | 1:A:81:VAL:HG11  | 1:A:79:LEU:HB2   | 7        | 1.18          |
| (1,150)  | 1:A:81:VAL:HG11  | 1:A:79:LEU:HB3   | 7        | 1.18          |
| (1,150)  | 1:A:81:VAL:HG12  | 1:A:79:LEU:HB2   | 7        | 1.18          |
| (1,150)  | 1:A:81:VAL:HG12  | 1:A:79:LEU:HB3   | 7        | 1.18          |
| (1,150)  | 1:A:81:VAL:HG13  | 1:A:79:LEU:HB2   | 7        | 1.18          |
| (1,150)  | 1:A:81:VAL:HG13  | 1:A:79:LEU:HB3   | 7        | 1.18          |
| (1,1431) | 1:B:118:PHE:HD1  | 1:B:118:PHE:H    | 6        | 1.18          |
| (1,1431) | 1:B:118:PHE:HD2  | 1:B:118:PHE:H    | 6        | 1.18          |
| (1,1311) | 1:B:108:GLN:HA   | 1:B:113:PHE:HE1  | 5        | 1.18          |
| (1,1311) | 1:B:108:GLN:HA   | 1:B:113:PHE:HE2  | 5        | 1.18          |
| (1,1232) | 1:B:100:VAL:HG11 | 1:B:102:GLY:H    | 5        | 1.18          |
| (1,1232) | 1:B:100:VAL:HG12 | 1:B:102:GLY:H    | 5        | 1.18          |
| (1,1232) | 1:B:100:VAL:HG13 | 1:B:102:GLY:H    | 5        | 1.18          |
| (1,109)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:H     | 3        | 1.18          |
| (1,109)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:H     | 3        | 1.18          |
| (1,109)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:H     | 3        | 1.18          |
| (1,1057) | 1:B:84:PHE:HE1   | 1:B:82:LYS:H     | 8        | 1.18          |
| (1,1057) | 1:B:84:PHE:HE2   | 1:B:82:LYS:H     | 8        | 1.18          |
| (1,1017) | 1:B:81:VAL:HG11  | 1:B:79:LEU:HB2   | 7        | 1.18          |
| (1,1017) | 1:B:81:VAL:HG11  | 1:B:79:LEU:HB3   | 7        | 1.18          |
| (1,1017) | 1:B:81:VAL:HG12  | 1:B:79:LEU:HB2   | 7        | 1.18          |
| (1,1017) | 1:B:81:VAL:HG12  | 1:B:79:LEU:HB3   | 7        | 1.18          |
| (1,1017) | 1:B:81:VAL:HG13  | 1:B:79:LEU:HB2   | 7        | 1.18          |
| (1,1017) | 1:B:81:VAL:HG13  | 1:B:79:LEU:HB3   | 7        | 1.18          |
| (1,966)  | 1:B:77:VAL:HG21  | 1:B:78:ASN:HB2   | 7        | 1.17          |
| (1,966)  | 1:B:77:VAL:HG22  | 1:B:78:ASN:HB2   | 7        | 1.17          |
| (1,966)  | 1:B:77:VAL:HG23  | 1:B:78:ASN:HB2   | 7        | 1.17          |
| (1,949)  | 1:B:77:VAL:HG21  | 1:B:68:MET:HA    | 4        | 1.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,949)  | 1:B:77:VAL:HG22  | 1:B:68:MET:HA    | 4        | 1.17          |
| (1,949)  | 1:B:77:VAL:HG23  | 1:B:68:MET:HA    | 4        | 1.17          |
| (1,873)  | 1:B:67:GLU:H     | 1:B:67:GLU:HG2   | 6        | 1.17          |
| (1,873)  | 1:B:67:GLU:H     | 1:B:67:GLU:HG3   | 6        | 1.17          |
| (1,82)   | 1:A:77:VAL:HG21  | 1:A:68:MET:HA    | 4        | 1.17          |
| (1,82)   | 1:A:77:VAL:HG22  | 1:A:68:MET:HA    | 4        | 1.17          |
| (1,82)   | 1:A:77:VAL:HG23  | 1:A:68:MET:HA    | 4        | 1.17          |
| (1,724)  | 1:A:133:ILE:HD11 | 1:A:134:THR:H    | 5        | 1.17          |
| (1,724)  | 1:A:133:ILE:HD12 | 1:A:134:THR:H    | 5        | 1.17          |
| (1,724)  | 1:A:133:ILE:HD13 | 1:A:134:THR:H    | 5        | 1.17          |
| (1,6)    | 1:A:67:GLU:H     | 1:A:67:GLU:HG2   | 6        | 1.17          |
| (1,6)    | 1:A:67:GLU:H     | 1:A:67:GLU:HG3   | 6        | 1.17          |
| (1,568)  | 1:A:119:HIS:HB3  | 1:A:101:HIS:HA   | 8        | 1.17          |
| (1,397)  | 1:A:103:LYS:HG2  | 1:A:116:ARG:H    | 5        | 1.17          |
| (1,397)  | 1:A:103:LYS:HG3  | 1:A:116:ARG:H    | 5        | 1.17          |
| (1,1750) | 1:A:115:SER:HB2  | 1:B:119:HIS:HE1  | 4        | 1.17          |
| (1,1435) | 1:B:119:HIS:HB3  | 1:B:101:HIS:HA   | 8        | 1.17          |
| (1,1264) | 1:B:103:LYS:HG2  | 1:B:116:ARG:H    | 5        | 1.17          |
| (1,1264) | 1:B:103:LYS:HG3  | 1:B:116:ARG:H    | 5        | 1.17          |
| (1,99)   | 1:A:77:VAL:HG21  | 1:A:78:ASN:HB2   | 7        | 1.16          |
| (1,99)   | 1:A:77:VAL:HG22  | 1:A:78:ASN:HB2   | 7        | 1.16          |
| (1,99)   | 1:A:77:VAL:HG23  | 1:A:78:ASN:HB2   | 7        | 1.16          |
| (1,976)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:H     | 5        | 1.16          |
| (1,976)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:H     | 5        | 1.16          |
| (1,976)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:H     | 5        | 1.16          |
| (1,920)  | 1:B:75:PHE:HE1   | 1:B:133:ILE:HD11 | 5        | 1.16          |
| (1,920)  | 1:B:75:PHE:HE1   | 1:B:133:ILE:HD12 | 5        | 1.16          |
| (1,920)  | 1:B:75:PHE:HE1   | 1:B:133:ILE:HD13 | 5        | 1.16          |
| (1,920)  | 1:B:75:PHE:HE2   | 1:B:133:ILE:HD11 | 5        | 1.16          |
| (1,920)  | 1:B:75:PHE:HE2   | 1:B:133:ILE:HD12 | 5        | 1.16          |
| (1,920)  | 1:B:75:PHE:HE2   | 1:B:133:ILE:HD13 | 5        | 1.16          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD11  | 1        | 1.16          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD12  | 1        | 1.16          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD13  | 1        | 1.16          |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD11  | 1        | 1.16          |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD12  | 1        | 1.16          |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD13  | 1        | 1.16          |
| (1,734)  | 1:A:135:SER:H    | 1:A:134:THR:HB   | 3        | 1.16          |
| (1,724)  | 1:A:133:ILE:HD11 | 1:A:134:THR:H    | 1        | 1.16          |
| (1,724)  | 1:A:133:ILE:HD12 | 1:A:134:THR:H    | 1        | 1.16          |
| (1,724)  | 1:A:133:ILE:HD13 | 1:A:134:THR:H    | 1        | 1.16          |
| (1,551)  | 1:A:118:PHE:HD1  | 1:A:103:LYS:HA   | 8        | 1.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,551)  | 1:A:118:PHE:HD2  | 1:A:103:LYS:HA   | 8        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD11  | 1        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD12  | 1        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD13  | 1        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD11  | 1        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD12  | 1        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD13  | 1        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD11  | 8        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD12  | 8        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD13  | 8        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD11  | 8        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD12  | 8        | 1.16          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD13  | 8        | 1.16          |
| (1,288)  | 1:A:93:VAL:HA    | 1:A:99:GLU:H     | 4        | 1.16          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD2   | 4        | 1.16          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD3   | 4        | 1.16          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD21  | 4        | 1.16          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD22  | 4        | 1.16          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD23  | 4        | 1.16          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD21  | 4        | 1.16          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD22  | 4        | 1.16          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD23  | 4        | 1.16          |
| (1,1761) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H    | 8        | 1.16          |
| (1,1761) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H    | 8        | 1.16          |
| (1,1750) | 1:A:115:SER:HB2  | 1:B:119:HIS:HE1  | 5        | 1.16          |
| (1,1740) | 1:A:113:PHE:HD1  | 1:B:121:LYS:H    | 9        | 1.16          |
| (1,1740) | 1:A:113:PHE:HD2  | 1:B:121:LYS:H    | 9        | 1.16          |
| (1,1601) | 1:B:135:SER:H    | 1:B:134:THR:HB   | 3        | 1.16          |
| (1,1591) | 1:B:133:ILE:HD11 | 1:B:134:THR:H    | 1        | 1.16          |
| (1,1591) | 1:B:133:ILE:HD12 | 1:B:134:THR:H    | 1        | 1.16          |
| (1,1591) | 1:B:133:ILE:HD13 | 1:B:134:THR:H    | 1        | 1.16          |
| (1,1482) | 1:B:124:ILE:HB   | 1:B:97:VAL:HA    | 6        | 1.16          |
| (1,1418) | 1:B:118:PHE:HD1  | 1:B:103:LYS:HA   | 8        | 1.16          |
| (1,1418) | 1:B:118:PHE:HD2  | 1:B:103:LYS:HA   | 8        | 1.16          |
| (1,1383) | 1:B:114:ILE:H    | 1:B:114:ILE:HG12 | 6        | 1.16          |
| (1,1155) | 1:B:93:VAL:HA    | 1:B:99:GLU:H     | 4        | 1.16          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD2   | 4        | 1.16          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD3   | 4        | 1.16          |
| (1,109)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:H     | 5        | 1.16          |
| (1,109)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:H     | 5        | 1.16          |
| (1,109)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:H     | 5        | 1.16          |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD21  | 4        | 1.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD22  | 4        | 1.16          |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD23  | 4        | 1.16          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD21  | 4        | 1.16          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD22  | 4        | 1.16          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD23  | 4        | 1.16          |
| (1,949)  | 1:B:77:VAL:HG21  | 1:B:68:MET:HA    | 9        | 1.15          |
| (1,949)  | 1:B:77:VAL:HG22  | 1:B:68:MET:HA    | 9        | 1.15          |
| (1,949)  | 1:B:77:VAL:HG23  | 1:B:68:MET:HA    | 9        | 1.15          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD11  | 8        | 1.15          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD12  | 8        | 1.15          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD13  | 8        | 1.15          |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD11  | 8        | 1.15          |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD12  | 8        | 1.15          |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD13  | 8        | 1.15          |
| (1,82)   | 1:A:77:VAL:HG21  | 1:A:68:MET:HA    | 1        | 1.15          |
| (1,82)   | 1:A:77:VAL:HG22  | 1:A:68:MET:HA    | 1        | 1.15          |
| (1,82)   | 1:A:77:VAL:HG23  | 1:A:68:MET:HA    | 1        | 1.15          |
| (1,82)   | 1:A:77:VAL:HG21  | 1:A:68:MET:HA    | 9        | 1.15          |
| (1,82)   | 1:A:77:VAL:HG22  | 1:A:68:MET:HA    | 9        | 1.15          |
| (1,82)   | 1:A:77:VAL:HG23  | 1:A:68:MET:HA    | 9        | 1.15          |
| (1,724)  | 1:A:133:ILE:HD11 | 1:A:134:THR:H    | 9        | 1.15          |
| (1,724)  | 1:A:133:ILE:HD12 | 1:A:134:THR:H    | 9        | 1.15          |
| (1,724)  | 1:A:133:ILE:HD13 | 1:A:134:THR:H    | 9        | 1.15          |
| (1,615)  | 1:A:124:ILE:HB   | 1:A:97:VAL:HA    | 6        | 1.15          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD11 | 9        | 1.15          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD12 | 9        | 1.15          |
| (1,603)  | 1:A:122:TYR:HA   | 1:A:124:ILE:HD13 | 9        | 1.15          |
| (1,53)   | 1:A:75:PHE:HE1   | 1:A:133:ILE:HD11 | 5        | 1.15          |
| (1,53)   | 1:A:75:PHE:HE1   | 1:A:133:ILE:HD12 | 5        | 1.15          |
| (1,53)   | 1:A:75:PHE:HE1   | 1:A:133:ILE:HD13 | 5        | 1.15          |
| (1,53)   | 1:A:75:PHE:HE2   | 1:A:133:ILE:HD11 | 5        | 1.15          |
| (1,53)   | 1:A:75:PHE:HE2   | 1:A:133:ILE:HD12 | 5        | 1.15          |
| (1,53)   | 1:A:75:PHE:HE2   | 1:A:133:ILE:HD13 | 5        | 1.15          |
| (1,516)  | 1:A:114:ILE:H    | 1:A:114:ILE:HG12 | 3        | 1.15          |
| (1,516)  | 1:A:114:ILE:H    | 1:A:114:ILE:HG12 | 6        | 1.15          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB2  | 8        | 1.15          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB3  | 8        | 1.15          |
| (1,365)  | 1:A:100:VAL:HG11 | 1:A:102:GLY:H    | 3        | 1.15          |
| (1,365)  | 1:A:100:VAL:HG12 | 1:A:102:GLY:H    | 3        | 1.15          |
| (1,365)  | 1:A:100:VAL:HG13 | 1:A:102:GLY:H    | 3        | 1.15          |
| (1,288)  | 1:A:93:VAL:HA    | 1:A:99:GLU:H     | 7        | 1.15          |
| (1,1736) | 1:A:111:HIS:HB2  | 1:B:122:TYR:HE1  | 2        | 1.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1736) | 1:A:111:HIS:HB2  | 1:B:122:TYR:HE2  | 2        | 1.15          |
| (1,1591) | 1:B:133:ILE:HD11 | 1:B:134:THR:H    | 9        | 1.15          |
| (1,1591) | 1:B:133:ILE:HD12 | 1:B:134:THR:H    | 9        | 1.15          |
| (1,1591) | 1:B:133:ILE:HD13 | 1:B:134:THR:H    | 9        | 1.15          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD11 | 9        | 1.15          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD12 | 9        | 1.15          |
| (1,1470) | 1:B:122:TYR:HA   | 1:B:124:ILE:HD13 | 9        | 1.15          |
| (1,1383) | 1:B:114:ILE:H    | 1:B:114:ILE:HG12 | 3        | 1.15          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB2  | 8        | 1.15          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB3  | 8        | 1.15          |
| (1,1232) | 1:B:100:VAL:HG11 | 1:B:102:GLY:H    | 3        | 1.15          |
| (1,1232) | 1:B:100:VAL:HG12 | 1:B:102:GLY:H    | 3        | 1.15          |
| (1,1232) | 1:B:100:VAL:HG13 | 1:B:102:GLY:H    | 3        | 1.15          |
| (1,1155) | 1:B:93:VAL:HA    | 1:B:99:GLU:H     | 7        | 1.15          |
| (1,949)  | 1:B:77:VAL:HG21  | 1:B:68:MET:HA    | 1        | 1.14          |
| (1,949)  | 1:B:77:VAL:HG22  | 1:B:68:MET:HA    | 1        | 1.14          |
| (1,949)  | 1:B:77:VAL:HG23  | 1:B:68:MET:HA    | 1        | 1.14          |
| (1,943)  | 1:B:76:SER:HB3   | 1:B:146:ASP:HA   | 3        | 1.14          |
| (1,906)  | 1:B:74:ARG:HG2   | 1:B:73:ASP:H     | 5        | 1.14          |
| (1,906)  | 1:B:74:ARG:HG3   | 1:B:73:ASP:H     | 5        | 1.14          |
| (1,76)   | 1:A:76:SER:HB3   | 1:A:146:ASP:HA   | 3        | 1.14          |
| (1,652)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HA   | 8        | 1.14          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG11  | 5        | 1.14          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG12  | 5        | 1.14          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG13  | 5        | 1.14          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG21  | 5        | 1.14          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG22  | 5        | 1.14          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG23  | 5        | 1.14          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB2  | 1        | 1.14          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB3  | 1        | 1.14          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB2  | 7        | 1.14          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB3  | 7        | 1.14          |
| (1,397)  | 1:A:103:LYS:HG2  | 1:A:116:ARG:H    | 7        | 1.14          |
| (1,397)  | 1:A:103:LYS:HG3  | 1:A:116:ARG:H    | 7        | 1.14          |
| (1,39)   | 1:A:74:ARG:HG2   | 1:A:73:ASP:H     | 5        | 1.14          |
| (1,39)   | 1:A:74:ARG:HG3   | 1:A:73:ASP:H     | 5        | 1.14          |
| (1,342)  | 1:A:98:ILE:HD11  | 1:A:122:TYR:HD1  | 4        | 1.14          |
| (1,342)  | 1:A:98:ILE:HD11  | 1:A:122:TYR:HD2  | 4        | 1.14          |
| (1,342)  | 1:A:98:ILE:HD12  | 1:A:122:TYR:HD1  | 4        | 1.14          |
| (1,342)  | 1:A:98:ILE:HD12  | 1:A:122:TYR:HD2  | 4        | 1.14          |
| (1,342)  | 1:A:98:ILE:HD13  | 1:A:122:TYR:HD1  | 4        | 1.14          |
| (1,342)  | 1:A:98:ILE:HD13  | 1:A:122:TYR:HD2  | 4        | 1.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1519) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HA  | 8        | 1.14          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG11 | 5        | 1.14          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG12 | 5        | 1.14          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG13 | 5        | 1.14          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG21 | 5        | 1.14          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG22 | 5        | 1.14          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG23 | 5        | 1.14          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB2 | 1        | 1.14          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB3 | 1        | 1.14          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB2 | 7        | 1.14          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB3 | 7        | 1.14          |
| (1,1264) | 1:B:103:LYS:HG2  | 1:B:116:ARG:H   | 7        | 1.14          |
| (1,1264) | 1:B:103:LYS:HG3  | 1:B:116:ARG:H   | 7        | 1.14          |
| (1,985)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB2 | 9        | 1.13          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD2 | 1        | 1.13          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD3 | 1        | 1.13          |
| (1,652)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HA  | 3        | 1.13          |
| (1,652)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HA  | 7        | 1.13          |
| (1,605)  | 1:A:123:ARG:HD2  | 1:A:98:ILE:H    | 8        | 1.13          |
| (1,605)  | 1:A:123:ARG:HD3  | 1:A:98:ILE:H    | 8        | 1.13          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD2 | 1        | 1.13          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD3 | 1        | 1.13          |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD1 | 4        | 1.13          |
| (1,165)  | 1:A:81:VAL:HG21  | 1:A:118:PHE:HD2 | 4        | 1.13          |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD1 | 4        | 1.13          |
| (1,165)  | 1:A:81:VAL:HG22  | 1:A:118:PHE:HD2 | 4        | 1.13          |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD1 | 4        | 1.13          |
| (1,165)  | 1:A:81:VAL:HG23  | 1:A:118:PHE:HD2 | 4        | 1.13          |
| (1,1595) | 1:B:133:ILE:HG12 | 1:B:147:GLY:HA2 | 2        | 1.13          |
| (1,1595) | 1:B:133:ILE:HG13 | 1:B:147:GLY:HA2 | 2        | 1.13          |
| (1,1519) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HA  | 3        | 1.13          |
| (1,1519) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HA  | 7        | 1.13          |
| (1,1472) | 1:B:123:ARG:HD2  | 1:B:98:ILE:H    | 8        | 1.13          |
| (1,1472) | 1:B:123:ARG:HD3  | 1:B:98:ILE:H    | 8        | 1.13          |
| (1,1374) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HD3 | 6        | 1.13          |
| (1,1374) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HD3 | 6        | 1.13          |
| (1,1374) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HD3 | 6        | 1.13          |
| (1,118)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB2 | 9        | 1.13          |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD1 | 4        | 1.13          |
| (1,1032) | 1:B:81:VAL:HG21  | 1:B:118:PHE:HD2 | 4        | 1.13          |
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD1 | 4        | 1.13          |
| (1,1032) | 1:B:81:VAL:HG22  | 1:B:118:PHE:HD2 | 4        | 1.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1032) | 1:B:81:VAL:HG23  | 1:B:118:PHE:HD1  | 4        | 1.13          |
| (1,1032) | 1:B:81:VAL:HG23  | 1:B:118:PHE:HD2  | 4        | 1.13          |
| (1,99)   | 1:A:77:VAL:HG21  | 1:A:78:ASN:HB2   | 1        | 1.12          |
| (1,99)   | 1:A:77:VAL:HG22  | 1:A:78:ASN:HB2   | 1        | 1.12          |
| (1,99)   | 1:A:77:VAL:HG23  | 1:A:78:ASN:HB2   | 1        | 1.12          |
| (1,966)  | 1:B:77:VAL:HG21  | 1:B:78:ASN:HB2   | 1        | 1.12          |
| (1,966)  | 1:B:77:VAL:HG22  | 1:B:78:ASN:HB2   | 1        | 1.12          |
| (1,966)  | 1:B:77:VAL:HG23  | 1:B:78:ASN:HB2   | 1        | 1.12          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD2  | 4        | 1.12          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD3  | 4        | 1.12          |
| (1,728)  | 1:A:133:ILE:HG12 | 1:A:147:GLY:HA2  | 2        | 1.12          |
| (1,728)  | 1:A:133:ILE:HG13 | 1:A:147:GLY:HA2  | 2        | 1.12          |
| (1,724)  | 1:A:133:ILE:HD11 | 1:A:134:THR:H    | 4        | 1.12          |
| (1,724)  | 1:A:133:ILE:HD12 | 1:A:134:THR:H    | 4        | 1.12          |
| (1,724)  | 1:A:133:ILE:HD13 | 1:A:134:THR:H    | 4        | 1.12          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG21 | 1        | 1.12          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG22 | 1        | 1.12          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG23 | 1        | 1.12          |
| (1,563)  | 1:A:118:PHE:HB2  | 1:A:118:PHE:H    | 8        | 1.12          |
| (1,539)  | 1:A:116:ARG:H    | 1:A:116:ARG:HG2  | 3        | 1.12          |
| (1,539)  | 1:A:116:ARG:H    | 1:A:116:ARG:HG3  | 3        | 1.12          |
| (1,507)  | 1:A:114:ILE:HD11 | 1:A:107:ARG:HD3  | 2        | 1.12          |
| (1,507)  | 1:A:114:ILE:HD12 | 1:A:107:ARG:HD3  | 2        | 1.12          |
| (1,507)  | 1:A:114:ILE:HD13 | 1:A:107:ARG:HD3  | 2        | 1.12          |
| (1,507)  | 1:A:114:ILE:HD11 | 1:A:107:ARG:HD3  | 5        | 1.12          |
| (1,507)  | 1:A:114:ILE:HD12 | 1:A:107:ARG:HD3  | 5        | 1.12          |
| (1,507)  | 1:A:114:ILE:HD13 | 1:A:107:ARG:HD3  | 5        | 1.12          |
| (1,457)  | 1:A:111:HIS:H    | 1:A:109:ASP:HB2  | 2        | 1.12          |
| (1,457)  | 1:A:111:HIS:H    | 1:A:109:ASP:HB3  | 2        | 1.12          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB2  | 3        | 1.12          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB3  | 3        | 1.12          |
| (1,301)  | 1:A:95:GLY:H     | 1:A:94:LEU:HG    | 1        | 1.12          |
| (1,301)  | 1:A:95:GLY:H     | 1:A:94:LEU:HG    | 3        | 1.12          |
| (1,236)  | 1:A:89:LEU:HD21  | 1:A:85:SER:HB3   | 4        | 1.12          |
| (1,236)  | 1:A:89:LEU:HD22  | 1:A:85:SER:HB3   | 4        | 1.12          |
| (1,236)  | 1:A:89:LEU:HD23  | 1:A:85:SER:HB3   | 4        | 1.12          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG12 | 4        | 1.12          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG13 | 4        | 1.12          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE1  | 5        | 1.12          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE2  | 5        | 1.12          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE1  | 5        | 1.12          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE2  | 5        | 1.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE1  | 5        | 1.12          |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE2  | 5        | 1.12          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD2  | 4        | 1.12          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD3  | 4        | 1.12          |
| (1,1591) | 1:B:133:ILE:HD11 | 1:B:134:THR:H    | 4        | 1.12          |
| (1,1591) | 1:B:133:ILE:HD12 | 1:B:134:THR:H    | 4        | 1.12          |
| (1,1591) | 1:B:133:ILE:HD13 | 1:B:134:THR:H    | 4        | 1.12          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG21 | 1        | 1.12          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG22 | 1        | 1.12          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG23 | 1        | 1.12          |
| (1,1430) | 1:B:118:PHE:HB2  | 1:B:118:PHE:H    | 8        | 1.12          |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG2  | 3        | 1.12          |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG3  | 3        | 1.12          |
| (1,1374) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HD3  | 1        | 1.12          |
| (1,1374) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HD3  | 1        | 1.12          |
| (1,1374) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HD3  | 1        | 1.12          |
| (1,1324) | 1:B:111:HIS:H    | 1:B:109:ASP:HB2  | 2        | 1.12          |
| (1,1324) | 1:B:111:HIS:H    | 1:B:109:ASP:HB3  | 2        | 1.12          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB2  | 3        | 1.12          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB3  | 3        | 1.12          |
| (1,1168) | 1:B:95:GLY:H     | 1:B:94:LEU:HG    | 1        | 1.12          |
| (1,1103) | 1:B:89:LEU:HD21  | 1:B:85:SER:HB3   | 4        | 1.12          |
| (1,1103) | 1:B:89:LEU:HD22  | 1:B:85:SER:HB3   | 4        | 1.12          |
| (1,1103) | 1:B:89:LEU:HD23  | 1:B:85:SER:HB3   | 4        | 1.12          |
| (1,880)  | 1:B:68:MET:HE1   | 1:B:122:TYR:HE1  | 2        | 1.11          |
| (1,880)  | 1:B:68:MET:HE1   | 1:B:122:TYR:HE2  | 2        | 1.11          |
| (1,880)  | 1:B:68:MET:HE2   | 1:B:122:TYR:HE1  | 2        | 1.11          |
| (1,880)  | 1:B:68:MET:HE2   | 1:B:122:TYR:HE2  | 2        | 1.11          |
| (1,880)  | 1:B:68:MET:HE3   | 1:B:122:TYR:HE1  | 2        | 1.11          |
| (1,880)  | 1:B:68:MET:HE3   | 1:B:122:TYR:HE2  | 2        | 1.11          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD2  | 5        | 1.11          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD3  | 5        | 1.11          |
| (1,724)  | 1:A:133:ILE:HD11 | 1:A:134:THR:H    | 7        | 1.11          |
| (1,724)  | 1:A:133:ILE:HD12 | 1:A:134:THR:H    | 7        | 1.11          |
| (1,724)  | 1:A:133:ILE:HD13 | 1:A:134:THR:H    | 7        | 1.11          |
| (1,563)  | 1:A:118:PHE:HB2  | 1:A:118:PHE:H    | 2        | 1.11          |
| (1,526)  | 1:A:115:SER:HA   | 1:A:114:ILE:HD11 | 4        | 1.11          |
| (1,526)  | 1:A:115:SER:HA   | 1:A:114:ILE:HD12 | 4        | 1.11          |
| (1,526)  | 1:A:115:SER:HA   | 1:A:114:ILE:HD13 | 4        | 1.11          |
| (1,507)  | 1:A:114:ILE:HD11 | 1:A:107:ARG:HD3  | 1        | 1.11          |
| (1,507)  | 1:A:114:ILE:HD12 | 1:A:107:ARG:HD3  | 1        | 1.11          |
| (1,507)  | 1:A:114:ILE:HD13 | 1:A:107:ARG:HD3  | 1        | 1.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,507)  | 1:A:114:ILE:HD11 | 1:A:107:ARG:HD3  | 6        | 1.11          |
| (1,507)  | 1:A:114:ILE:HD12 | 1:A:107:ARG:HD3  | 6        | 1.11          |
| (1,507)  | 1:A:114:ILE:HD13 | 1:A:107:ARG:HD3  | 6        | 1.11          |
| (1,238)  | 1:A:89:LEU:HD11  | 1:A:85:SER:H     | 1        | 1.11          |
| (1,238)  | 1:A:89:LEU:HD12  | 1:A:85:SER:H     | 1        | 1.11          |
| (1,238)  | 1:A:89:LEU:HD13  | 1:A:85:SER:H     | 1        | 1.11          |
| (1,1770) | 1:A:123:ARG:HD2  | 1:B:113:PHE:H    | 8        | 1.11          |
| (1,1770) | 1:A:123:ARG:HD3  | 1:B:113:PHE:H    | 8        | 1.11          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD2  | 5        | 1.11          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD3  | 5        | 1.11          |
| (1,1591) | 1:B:133:ILE:HD11 | 1:B:134:THR:H    | 7        | 1.11          |
| (1,1591) | 1:B:133:ILE:HD12 | 1:B:134:THR:H    | 7        | 1.11          |
| (1,1591) | 1:B:133:ILE:HD13 | 1:B:134:THR:H    | 7        | 1.11          |
| (1,1430) | 1:B:118:PHE:HB2  | 1:B:118:PHE:H    | 2        | 1.11          |
| (1,1393) | 1:B:115:SER:HA   | 1:B:114:ILE:HD11 | 4        | 1.11          |
| (1,1393) | 1:B:115:SER:HA   | 1:B:114:ILE:HD12 | 4        | 1.11          |
| (1,1393) | 1:B:115:SER:HA   | 1:B:114:ILE:HD13 | 4        | 1.11          |
| (1,1374) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HD3  | 2        | 1.11          |
| (1,1374) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HD3  | 2        | 1.11          |
| (1,1374) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HD3  | 2        | 1.11          |
| (1,1374) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HD3  | 5        | 1.11          |
| (1,1374) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HD3  | 5        | 1.11          |
| (1,1374) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HD3  | 5        | 1.11          |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB2   | 2        | 1.11          |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB3   | 2        | 1.11          |
| (1,1168) | 1:B:95:GLY:H     | 1:B:94:LEU:HG    | 3        | 1.11          |
| (1,1105) | 1:B:89:LEU:HD11  | 1:B:85:SER:H     | 1        | 1.11          |
| (1,1105) | 1:B:89:LEU:HD12  | 1:B:85:SER:H     | 1        | 1.11          |
| (1,1105) | 1:B:89:LEU:HD13  | 1:B:85:SER:H     | 1        | 1.11          |
| (1,652)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HA   | 6        | 1.1           |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB2  | 7        | 1.1           |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB3  | 7        | 1.1           |
| (1,517)  | 1:A:114:ILE:H    | 1:A:114:ILE:HG13 | 8        | 1.1           |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG21 | 6        | 1.1           |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG22 | 6        | 1.1           |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG23 | 6        | 1.1           |
| (1,367)  | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB2   | 2        | 1.1           |
| (1,367)  | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB3   | 2        | 1.1           |
| (1,288)  | 1:A:93:VAL:HA    | 1:A:99:GLU:H     | 6        | 1.1           |
| (1,260)  | 1:A:89:LEU:HD21  | 1:A:103:LYS:H    | 4        | 1.1           |
| (1,260)  | 1:A:89:LEU:HD22  | 1:A:103:LYS:H    | 4        | 1.1           |
| (1,260)  | 1:A:89:LEU:HD23  | 1:A:103:LYS:H    | 4        | 1.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1591) | 1:B:133:ILE:HD11 | 1:B:134:THR:H    | 6        | 1.1           |
| (1,1591) | 1:B:133:ILE:HD12 | 1:B:134:THR:H    | 6        | 1.1           |
| (1,1591) | 1:B:133:ILE:HD13 | 1:B:134:THR:H    | 6        | 1.1           |
| (1,1591) | 1:B:133:ILE:HD11 | 1:B:134:THR:H    | 8        | 1.1           |
| (1,1591) | 1:B:133:ILE:HD12 | 1:B:134:THR:H    | 8        | 1.1           |
| (1,1591) | 1:B:133:ILE:HD13 | 1:B:134:THR:H    | 8        | 1.1           |
| (1,1519) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HA   | 6        | 1.1           |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB2  | 7        | 1.1           |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB3  | 7        | 1.1           |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG21 | 6        | 1.1           |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG22 | 6        | 1.1           |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG23 | 6        | 1.1           |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE1  | 2        | 1.1           |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE2  | 2        | 1.1           |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE1  | 2        | 1.1           |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE2  | 2        | 1.1           |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE1  | 2        | 1.1           |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE2  | 2        | 1.1           |
| (1,1155) | 1:B:93:VAL:HA    | 1:B:99:GLU:H     | 6        | 1.1           |
| (1,1127) | 1:B:89:LEU:HD21  | 1:B:103:LYS:H    | 4        | 1.1           |
| (1,1127) | 1:B:89:LEU:HD22  | 1:B:103:LYS:H    | 4        | 1.1           |
| (1,1127) | 1:B:89:LEU:HD23  | 1:B:103:LYS:H    | 4        | 1.1           |
| (1,943)  | 1:B:76:SER:HB3   | 1:B:146:ASP:HA   | 8        | 1.09          |
| (1,936)  | 1:B:76:SER:HB3   | 1:B:146:ASP:HA   | 3        | 1.09          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD2  | 3        | 1.09          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD3  | 3        | 1.09          |
| (1,841)  | 1:A:147:GLY:HA2  | 1:A:132:THR:HA   | 2        | 1.09          |
| (1,76)   | 1:A:76:SER:HB3   | 1:A:146:ASP:HA   | 8        | 1.09          |
| (1,724)  | 1:A:133:ILE:HD11 | 1:A:134:THR:H    | 6        | 1.09          |
| (1,724)  | 1:A:133:ILE:HD12 | 1:A:134:THR:H    | 6        | 1.09          |
| (1,724)  | 1:A:133:ILE:HD13 | 1:A:134:THR:H    | 6        | 1.09          |
| (1,724)  | 1:A:133:ILE:HD11 | 1:A:134:THR:H    | 8        | 1.09          |
| (1,724)  | 1:A:133:ILE:HD12 | 1:A:134:THR:H    | 8        | 1.09          |
| (1,724)  | 1:A:133:ILE:HD13 | 1:A:134:THR:H    | 8        | 1.09          |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE1   | 6        | 1.09          |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE2   | 6        | 1.09          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE1   | 6        | 1.09          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE2   | 6        | 1.09          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE1   | 6        | 1.09          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE2   | 6        | 1.09          |
| (1,69)   | 1:A:76:SER:HB3   | 1:A:146:ASP:HA   | 3        | 1.09          |
| (1,652)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HA   | 1        | 1.09          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,652)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HA   | 2        | 1.09          |
| (1,652)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HA   | 4        | 1.09          |
| (1,652)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HA   | 9        | 1.09          |
| (1,516)  | 1:A:114:ILE:H    | 1:A:114:ILE:HG12 | 5        | 1.09          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB2  | 4        | 1.09          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB3  | 4        | 1.09          |
| (1,260)  | 1:A:89:LEU:HD21  | 1:A:103:LYS:H    | 7        | 1.09          |
| (1,260)  | 1:A:89:LEU:HD22  | 1:A:103:LYS:H    | 7        | 1.09          |
| (1,260)  | 1:A:89:LEU:HD23  | 1:A:103:LYS:H    | 7        | 1.09          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD2  | 3        | 1.09          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD3  | 3        | 1.09          |
| (1,1708) | 1:B:147:GLY:HA2  | 1:B:132:THR:HA   | 2        | 1.09          |
| (1,170)  | 1:A:83:HIS:H     | 1:A:81:VAL:HB    | 6        | 1.09          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE1   | 6        | 1.09          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE2   | 6        | 1.09          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE1   | 6        | 1.09          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE2   | 6        | 1.09          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE1   | 6        | 1.09          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE2   | 6        | 1.09          |
| (1,1519) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HA   | 1        | 1.09          |
| (1,1519) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HA   | 2        | 1.09          |
| (1,1519) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HA   | 4        | 1.09          |
| (1,1519) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HA   | 9        | 1.09          |
| (1,1384) | 1:B:114:ILE:H    | 1:B:114:ILE:HG13 | 8        | 1.09          |
| (1,1383) | 1:B:114:ILE:H    | 1:B:114:ILE:HG12 | 5        | 1.09          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB2  | 4        | 1.09          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB3  | 4        | 1.09          |
| (1,1127) | 1:B:89:LEU:HD21  | 1:B:103:LYS:H    | 7        | 1.09          |
| (1,1127) | 1:B:89:LEU:HD22  | 1:B:103:LYS:H    | 7        | 1.09          |
| (1,1127) | 1:B:89:LEU:HD23  | 1:B:103:LYS:H    | 7        | 1.09          |
| (1,1103) | 1:B:89:LEU:HD21  | 1:B:85:SER:HB3   | 8        | 1.09          |
| (1,1103) | 1:B:89:LEU:HD22  | 1:B:85:SER:HB3   | 8        | 1.09          |
| (1,1103) | 1:B:89:LEU:HD23  | 1:B:85:SER:HB3   | 8        | 1.09          |
| (1,1037) | 1:B:83:HIS:H     | 1:B:81:VAL:HB    | 6        | 1.09          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG2   | 2        | 1.08          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG3   | 2        | 1.08          |
| (1,652)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HA   | 5        | 1.08          |
| (1,507)  | 1:A:114:ILE:HD11 | 1:A:107:ARG:HD3  | 3        | 1.08          |
| (1,507)  | 1:A:114:ILE:HD12 | 1:A:107:ARG:HD3  | 3        | 1.08          |
| (1,507)  | 1:A:114:ILE:HD13 | 1:A:107:ARG:HD3  | 3        | 1.08          |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG21 | 5        | 1.08          |
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG22 | 5        | 1.08          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,440)  | 1:A:107:ARG:HB2  | 1:A:114:ILE:HG23 | 5        | 1.08          |
| (1,296)  | 1:A:94:LEU:H     | 1:A:99:GLU:H     | 8        | 1.08          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD2   | 8        | 1.08          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD3   | 8        | 1.08          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG2   | 2        | 1.08          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG3   | 2        | 1.08          |
| (1,236)  | 1:A:89:LEU:HD21  | 1:A:85:SER:HB3   | 8        | 1.08          |
| (1,236)  | 1:A:89:LEU:HD22  | 1:A:85:SER:HB3   | 8        | 1.08          |
| (1,236)  | 1:A:89:LEU:HD23  | 1:A:85:SER:HB3   | 8        | 1.08          |
| (1,1767) | 1:A:122:TYR:HB2  | 1:B:112:GLY:HA3  | 4        | 1.08          |
| (1,1767) | 1:A:122:TYR:HB3  | 1:B:112:GLY:HA3  | 4        | 1.08          |
| (1,1519) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HA   | 5        | 1.08          |
| (1,1374) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HD3  | 3        | 1.08          |
| (1,1374) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HD3  | 3        | 1.08          |
| (1,1374) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HD3  | 3        | 1.08          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG21 | 5        | 1.08          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG22 | 5        | 1.08          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG23 | 5        | 1.08          |
| (1,1163) | 1:B:94:LEU:H     | 1:B:99:GLU:H     | 8        | 1.08          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD2   | 8        | 1.08          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD3   | 8        | 1.08          |
| (1,978)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HE1  | 3        | 1.07          |
| (1,978)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HE2  | 3        | 1.07          |
| (1,978)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HE1  | 3        | 1.07          |
| (1,978)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HE2  | 3        | 1.07          |
| (1,978)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HE1  | 3        | 1.07          |
| (1,978)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HE2  | 3        | 1.07          |
| (1,857)  | 1:A:150:LYS:H    | 1:A:150:LYS:HD2  | 2        | 1.07          |
| (1,857)  | 1:A:150:LYS:H    | 1:A:150:LYS:HD3  | 2        | 1.07          |
| (1,857)  | 1:A:150:LYS:H    | 1:A:150:LYS:HD2  | 8        | 1.07          |
| (1,857)  | 1:A:150:LYS:H    | 1:A:150:LYS:HD3  | 8        | 1.07          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD2  | 7        | 1.07          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD3  | 7        | 1.07          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD2  | 9        | 1.07          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD3  | 9        | 1.07          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG21 | 6        | 1.07          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG22 | 6        | 1.07          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG23 | 6        | 1.07          |
| (1,365)  | 1:A:100:VAL:HG11 | 1:A:102:GLY:H    | 8        | 1.07          |
| (1,365)  | 1:A:100:VAL:HG12 | 1:A:102:GLY:H    | 8        | 1.07          |
| (1,365)  | 1:A:100:VAL:HG13 | 1:A:102:GLY:H    | 8        | 1.07          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD11  | 1        | 1.07          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD12  | 1        | 1.07          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD13  | 1        | 1.07          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD21  | 1        | 1.07          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD22  | 1        | 1.07          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD23  | 1        | 1.07          |
| (1,1745) | 1:A:114:ILE:H    | 1:B:121:LYS:H    | 8        | 1.07          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD2  | 2        | 1.07          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD3  | 2        | 1.07          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD2  | 8        | 1.07          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD3  | 8        | 1.07          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD2  | 7        | 1.07          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD3  | 7        | 1.07          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD2  | 9        | 1.07          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD3  | 9        | 1.07          |
| (1,166)  | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD1  | 8        | 1.07          |
| (1,166)  | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD2  | 8        | 1.07          |
| (1,166)  | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD1  | 8        | 1.07          |
| (1,166)  | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD2  | 8        | 1.07          |
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD1  | 8        | 1.07          |
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD2  | 8        | 1.07          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG21 | 6        | 1.07          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG22 | 6        | 1.07          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG23 | 6        | 1.07          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG21 | 8        | 1.07          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG22 | 8        | 1.07          |
| (1,1307) | 1:B:107:ARG:HB2  | 1:B:114:ILE:HG23 | 8        | 1.07          |
| (1,1232) | 1:B:100:VAL:HG11 | 1:B:102:GLY:H    | 8        | 1.07          |
| (1,1232) | 1:B:100:VAL:HG12 | 1:B:102:GLY:H    | 8        | 1.07          |
| (1,1232) | 1:B:100:VAL:HG13 | 1:B:102:GLY:H    | 8        | 1.07          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD11  | 1        | 1.07          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD12  | 1        | 1.07          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD13  | 1        | 1.07          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD21  | 1        | 1.07          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD22  | 1        | 1.07          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD23  | 1        | 1.07          |
| (1,1155) | 1:B:93:VAL:HA    | 1:B:99:GLU:H     | 3        | 1.07          |
| (1,111)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HE1  | 3        | 1.07          |
| (1,111)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HE2  | 3        | 1.07          |
| (1,111)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HE1  | 3        | 1.07          |
| (1,111)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HE2  | 3        | 1.07          |
| (1,111)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HE1  | 3        | 1.07          |
| (1,111)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HE2  | 3        | 1.07          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1033) | 1:B:81:VAL:HG11 | 1:B:118:PHE:HD1  | 8        | 1.07          |
| (1,1033) | 1:B:81:VAL:HG11 | 1:B:118:PHE:HD2  | 8        | 1.07          |
| (1,1033) | 1:B:81:VAL:HG12 | 1:B:118:PHE:HD1  | 8        | 1.07          |
| (1,1033) | 1:B:81:VAL:HG12 | 1:B:118:PHE:HD2  | 8        | 1.07          |
| (1,1033) | 1:B:81:VAL:HG13 | 1:B:118:PHE:HD1  | 8        | 1.07          |
| (1,1033) | 1:B:81:VAL:HG13 | 1:B:118:PHE:HD2  | 8        | 1.07          |
| (1,99)   | 1:A:77:VAL:HG21 | 1:A:78:ASN:HB2   | 2        | 1.06          |
| (1,99)   | 1:A:77:VAL:HG22 | 1:A:78:ASN:HB2   | 2        | 1.06          |
| (1,99)   | 1:A:77:VAL:HG23 | 1:A:78:ASN:HB2   | 2        | 1.06          |
| (1,966)  | 1:B:77:VAL:HG21 | 1:B:78:ASN:HB2   | 2        | 1.06          |
| (1,966)  | 1:B:77:VAL:HG22 | 1:B:78:ASN:HB2   | 2        | 1.06          |
| (1,966)  | 1:B:77:VAL:HG23 | 1:B:78:ASN:HB2   | 2        | 1.06          |
| (1,943)  | 1:B:76:SER:HB3  | 1:B:146:ASP:HA   | 4        | 1.06          |
| (1,843)  | 1:A:147:GLY:HA2 | 1:A:133:ILE:HB   | 4        | 1.06          |
| (1,76)   | 1:A:76:SER:HB3  | 1:A:146:ASP:HA   | 4        | 1.06          |
| (1,459)  | 1:A:111:HIS:H   | 1:A:110:GLU:H    | 6        | 1.06          |
| (1,458)  | 1:A:111:HIS:H   | 1:A:110:GLU:H    | 6        | 1.06          |
| (1,440)  | 1:A:107:ARG:HB2 | 1:A:114:ILE:HG21 | 8        | 1.06          |
| (1,440)  | 1:A:107:ARG:HB2 | 1:A:114:ILE:HG22 | 8        | 1.06          |
| (1,440)  | 1:A:107:ARG:HB2 | 1:A:114:ILE:HG23 | 8        | 1.06          |
| (1,321)  | 1:A:97:VAL:H    | 1:A:93:VAL:HB    | 9        | 1.06          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD11  | 3        | 1.06          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD12  | 3        | 1.06          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD13  | 3        | 1.06          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD21  | 3        | 1.06          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD22  | 3        | 1.06          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD23  | 3        | 1.06          |
| (1,288)  | 1:A:93:VAL:HA   | 1:A:99:GLU:H     | 3        | 1.06          |
| (1,188)  | 1:A:83:HIS:H    | 1:A:141:GLY:HA2  | 5        | 1.06          |
| (1,1760) | 1:A:120:ARG:HB2 | 1:B:111:HIS:H    | 3        | 1.06          |
| (1,1760) | 1:A:120:ARG:HB3 | 1:B:111:HIS:H    | 3        | 1.06          |
| (1,1710) | 1:B:147:GLY:HA2 | 1:B:133:ILE:HB   | 4        | 1.06          |
| (1,1482) | 1:B:124:ILE:HB  | 1:B:97:VAL:HA    | 1        | 1.06          |
| (1,1326) | 1:B:111:HIS:H   | 1:B:110:GLU:H    | 6        | 1.06          |
| (1,1325) | 1:B:111:HIS:H   | 1:B:110:GLU:H    | 6        | 1.06          |
| (1,1188) | 1:B:97:VAL:H    | 1:B:93:VAL:HB    | 9        | 1.06          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD11  | 3        | 1.06          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD12  | 3        | 1.06          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD13  | 3        | 1.06          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD21  | 3        | 1.06          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD22  | 3        | 1.06          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD23  | 3        | 1.06          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1055) | 1:B:83:HIS:H    | 1:B:141:GLY:HA2  | 5        | 1.06          |
| (1,978)  | 1:B:77:VAL:HG11 | 1:B:122:TYR:HE1  | 7        | 1.05          |
| (1,978)  | 1:B:77:VAL:HG11 | 1:B:122:TYR:HE2  | 7        | 1.05          |
| (1,978)  | 1:B:77:VAL:HG12 | 1:B:122:TYR:HE1  | 7        | 1.05          |
| (1,978)  | 1:B:77:VAL:HG12 | 1:B:122:TYR:HE2  | 7        | 1.05          |
| (1,978)  | 1:B:77:VAL:HG13 | 1:B:122:TYR:HE1  | 7        | 1.05          |
| (1,978)  | 1:B:77:VAL:HG13 | 1:B:122:TYR:HE2  | 7        | 1.05          |
| (1,949)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HA    | 5        | 1.05          |
| (1,949)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HA    | 5        | 1.05          |
| (1,949)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HA    | 5        | 1.05          |
| (1,849)  | 1:A:147:GLY:HA2 | 1:A:148:PRO:HD2  | 2        | 1.05          |
| (1,849)  | 1:A:147:GLY:HA2 | 1:A:148:PRO:HD3  | 2        | 1.05          |
| (1,841)  | 1:A:147:GLY:HA2 | 1:A:132:THR:HA   | 3        | 1.05          |
| (1,82)   | 1:A:77:VAL:HG21 | 1:A:68:MET:HA    | 5        | 1.05          |
| (1,82)   | 1:A:77:VAL:HG22 | 1:A:68:MET:HA    | 5        | 1.05          |
| (1,82)   | 1:A:77:VAL:HG23 | 1:A:68:MET:HA    | 5        | 1.05          |
| (1,615)  | 1:A:124:ILE:HB  | 1:A:97:VAL:HA    | 1        | 1.05          |
| (1,600)  | 1:A:122:TYR:HA  | 1:A:123:ARG:HB3  | 7        | 1.05          |
| (1,563)  | 1:A:118:PHE:HB2 | 1:A:118:PHE:H    | 6        | 1.05          |
| (1,527)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD11 | 8        | 1.05          |
| (1,527)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD12 | 8        | 1.05          |
| (1,527)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD13 | 8        | 1.05          |
| (1,526)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD11 | 8        | 1.05          |
| (1,526)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD12 | 8        | 1.05          |
| (1,526)  | 1:A:115:SER:HA  | 1:A:114:ILE:HD13 | 8        | 1.05          |
| (1,453)  | 1:A:110:GLU:H   | 1:A:109:ASP:HB2  | 9        | 1.05          |
| (1,453)  | 1:A:110:GLU:H   | 1:A:109:ASP:HB3  | 9        | 1.05          |
| (1,440)  | 1:A:107:ARG:HB2 | 1:A:114:ILE:HG21 | 7        | 1.05          |
| (1,440)  | 1:A:107:ARG:HB2 | 1:A:114:ILE:HG22 | 7        | 1.05          |
| (1,440)  | 1:A:107:ARG:HB2 | 1:A:114:ILE:HG23 | 7        | 1.05          |
| (1,1716) | 1:B:147:GLY:HA2 | 1:B:148:PRO:HD2  | 2        | 1.05          |
| (1,1716) | 1:B:147:GLY:HA2 | 1:B:148:PRO:HD3  | 2        | 1.05          |
| (1,1708) | 1:B:147:GLY:HA2 | 1:B:132:THR:HA   | 3        | 1.05          |
| (1,1467) | 1:B:122:TYR:HA  | 1:B:123:ARG:HB3  | 7        | 1.05          |
| (1,1430) | 1:B:118:PHE:HB2 | 1:B:118:PHE:H    | 6        | 1.05          |
| (1,1394) | 1:B:115:SER:HA  | 1:B:114:ILE:HD11 | 8        | 1.05          |
| (1,1394) | 1:B:115:SER:HA  | 1:B:114:ILE:HD12 | 8        | 1.05          |
| (1,1394) | 1:B:115:SER:HA  | 1:B:114:ILE:HD13 | 8        | 1.05          |
| (1,1393) | 1:B:115:SER:HA  | 1:B:114:ILE:HD11 | 8        | 1.05          |
| (1,1393) | 1:B:115:SER:HA  | 1:B:114:ILE:HD12 | 8        | 1.05          |
| (1,1393) | 1:B:115:SER:HA  | 1:B:114:ILE:HD13 | 8        | 1.05          |
| (1,1320) | 1:B:110:GLU:H   | 1:B:109:ASP:HB2  | 9        | 1.05          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1320) | 1:B:110:GLU:H   | 1:B:109:ASP:HB3  | 9        | 1.05          |
| (1,111)  | 1:A:77:VAL:HG11 | 1:A:122:TYR:HE1  | 7        | 1.05          |
| (1,111)  | 1:A:77:VAL:HG11 | 1:A:122:TYR:HE2  | 7        | 1.05          |
| (1,111)  | 1:A:77:VAL:HG12 | 1:A:122:TYR:HE1  | 7        | 1.05          |
| (1,111)  | 1:A:77:VAL:HG12 | 1:A:122:TYR:HE2  | 7        | 1.05          |
| (1,111)  | 1:A:77:VAL:HG13 | 1:A:122:TYR:HE1  | 7        | 1.05          |
| (1,111)  | 1:A:77:VAL:HG13 | 1:A:122:TYR:HE2  | 7        | 1.05          |
| (1,936)  | 1:B:76:SER:HB3  | 1:B:146:ASP:HA   | 8        | 1.04          |
| (1,861)  | 1:A:150:LYS:HA  | 1:A:151:GLN:H    | 8        | 1.04          |
| (1,841)  | 1:A:147:GLY:HA2 | 1:A:132:THR:HA   | 8        | 1.04          |
| (1,69)   | 1:A:76:SER:HB3  | 1:A:146:ASP:HA   | 8        | 1.04          |
| (1,524)  | 1:A:115:SER:HB2 | 1:A:106:GLU:H    | 7        | 1.04          |
| (1,506)  | 1:A:114:ILE:HB  | 1:A:107:ARG:HD3  | 5        | 1.04          |
| (1,1761) | 1:A:120:ARG:HB2 | 1:B:111:HIS:H    | 4        | 1.04          |
| (1,1761) | 1:A:120:ARG:HB3 | 1:B:111:HIS:H    | 4        | 1.04          |
| (1,1728) | 1:B:150:LYS:HA  | 1:B:151:GLN:H    | 8        | 1.04          |
| (1,1710) | 1:B:147:GLY:HA2 | 1:B:133:ILE:HB   | 6        | 1.04          |
| (1,1708) | 1:B:147:GLY:HA2 | 1:B:132:THR:HA   | 8        | 1.04          |
| (1,170)  | 1:A:83:HIS:H    | 1:A:81:VAL:HB    | 8        | 1.04          |
| (1,150)  | 1:A:81:VAL:HG11 | 1:A:79:LEU:HB2   | 1        | 1.04          |
| (1,150)  | 1:A:81:VAL:HG11 | 1:A:79:LEU:HB3   | 1        | 1.04          |
| (1,150)  | 1:A:81:VAL:HG12 | 1:A:79:LEU:HB2   | 1        | 1.04          |
| (1,150)  | 1:A:81:VAL:HG12 | 1:A:79:LEU:HB3   | 1        | 1.04          |
| (1,150)  | 1:A:81:VAL:HG13 | 1:A:79:LEU:HB2   | 1        | 1.04          |
| (1,150)  | 1:A:81:VAL:HG13 | 1:A:79:LEU:HB3   | 1        | 1.04          |
| (1,1391) | 1:B:115:SER:HB2 | 1:B:106:GLU:H    | 7        | 1.04          |
| (1,1373) | 1:B:114:ILE:HB  | 1:B:107:ARG:HD3  | 5        | 1.04          |
| (1,1307) | 1:B:107:ARG:HB2 | 1:B:114:ILE:HG21 | 7        | 1.04          |
| (1,1307) | 1:B:107:ARG:HB2 | 1:B:114:ILE:HG22 | 7        | 1.04          |
| (1,1307) | 1:B:107:ARG:HB2 | 1:B:114:ILE:HG23 | 7        | 1.04          |
| (1,1209) | 1:B:98:ILE:HD11 | 1:B:122:TYR:HD1  | 4        | 1.04          |
| (1,1209) | 1:B:98:ILE:HD11 | 1:B:122:TYR:HD2  | 4        | 1.04          |
| (1,1209) | 1:B:98:ILE:HD12 | 1:B:122:TYR:HD1  | 4        | 1.04          |
| (1,1209) | 1:B:98:ILE:HD12 | 1:B:122:TYR:HD2  | 4        | 1.04          |
| (1,1209) | 1:B:98:ILE:HD13 | 1:B:122:TYR:HD1  | 4        | 1.04          |
| (1,1209) | 1:B:98:ILE:HD13 | 1:B:122:TYR:HD2  | 4        | 1.04          |
| (1,1037) | 1:B:83:HIS:H    | 1:B:81:VAL:HB    | 8        | 1.04          |
| (1,1017) | 1:B:81:VAL:HG11 | 1:B:79:LEU:HB2   | 1        | 1.04          |
| (1,1017) | 1:B:81:VAL:HG11 | 1:B:79:LEU:HB3   | 1        | 1.04          |
| (1,1017) | 1:B:81:VAL:HG12 | 1:B:79:LEU:HB2   | 1        | 1.04          |
| (1,1017) | 1:B:81:VAL:HG12 | 1:B:79:LEU:HB3   | 1        | 1.04          |
| (1,1017) | 1:B:81:VAL:HG13 | 1:B:79:LEU:HB2   | 1        | 1.04          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1017) | 1:B:81:VAL:HG13  | 1:B:79:LEU:HB3   | 1        | 1.04          |
| (1,976)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:H     | 8        | 1.03          |
| (1,976)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:H     | 8        | 1.03          |
| (1,976)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:H     | 8        | 1.03          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD2  | 8        | 1.03          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD3  | 8        | 1.03          |
| (1,843)  | 1:A:147:GLY:HA2  | 1:A:133:ILE:HB   | 6        | 1.03          |
| (1,813)  | 1:A:145:VAL:HA   | 1:A:135:SER:H    | 5        | 1.03          |
| (1,563)  | 1:A:118:PHE:HB2  | 1:A:118:PHE:H    | 1        | 1.03          |
| (1,1430) | 1:B:118:PHE:HB2  | 1:B:118:PHE:H    | 1        | 1.03          |
| (1,109)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:H     | 8        | 1.03          |
| (1,109)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:H     | 8        | 1.03          |
| (1,109)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:H     | 8        | 1.03          |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG2   | 6        | 1.03          |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG3   | 6        | 1.03          |
| (1,981)  | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG11 | 2        | 1.02          |
| (1,981)  | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG12 | 2        | 1.02          |
| (1,981)  | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG13 | 2        | 1.02          |
| (1,981)  | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG11 | 2        | 1.02          |
| (1,981)  | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG12 | 2        | 1.02          |
| (1,981)  | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG13 | 2        | 1.02          |
| (1,981)  | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG11 | 2        | 1.02          |
| (1,981)  | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG12 | 2        | 1.02          |
| (1,981)  | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG13 | 2        | 1.02          |
| (1,598)  | 1:A:122:TYR:HB2  | 1:A:122:TYR:H    | 9        | 1.02          |
| (1,598)  | 1:A:122:TYR:HB3  | 1:A:122:TYR:H    | 9        | 1.02          |
| (1,597)  | 1:A:122:TYR:HB2  | 1:A:122:TYR:H    | 9        | 1.02          |
| (1,597)  | 1:A:122:TYR:HB3  | 1:A:122:TYR:H    | 9        | 1.02          |
| (1,365)  | 1:A:100:VAL:HG11 | 1:A:102:GLY:H    | 6        | 1.02          |
| (1,365)  | 1:A:100:VAL:HG12 | 1:A:102:GLY:H    | 6        | 1.02          |
| (1,365)  | 1:A:100:VAL:HG13 | 1:A:102:GLY:H    | 6        | 1.02          |
| (1,288)  | 1:A:93:VAL:HA    | 1:A:99:GLU:H     | 5        | 1.02          |
| (1,246)  | 1:A:89:LEU:H     | 1:A:89:LEU:HG    | 3        | 1.02          |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG2   | 6        | 1.02          |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG3   | 6        | 1.02          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG12 | 6        | 1.02          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG13 | 6        | 1.02          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD2  | 8        | 1.02          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD3  | 8        | 1.02          |
| (1,1680) | 1:B:145:VAL:HA   | 1:B:135:SER:H    | 5        | 1.02          |
| (1,1465) | 1:B:122:TYR:HB2  | 1:B:122:TYR:H    | 9        | 1.02          |
| (1,1465) | 1:B:122:TYR:HB3  | 1:B:122:TYR:H    | 9        | 1.02          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1464) | 1:B:122:TYR:HB2  | 1:B:122:TYR:H   | 9        | 1.02          |
| (1,1464) | 1:B:122:TYR:HB3  | 1:B:122:TYR:H   | 9        | 1.02          |
| (1,1232) | 1:B:100:VAL:HG11 | 1:B:102:GLY:H   | 6        | 1.02          |
| (1,1232) | 1:B:100:VAL:HG12 | 1:B:102:GLY:H   | 6        | 1.02          |
| (1,1232) | 1:B:100:VAL:HG13 | 1:B:102:GLY:H   | 6        | 1.02          |
| (1,1155) | 1:B:93:VAL:HA    | 1:B:99:GLU:H    | 5        | 1.02          |
| (1,1113) | 1:B:89:LEU:H     | 1:B:89:LEU:HG   | 3        | 1.02          |
| (1,936)  | 1:B:76:SER:HB3   | 1:B:146:ASP:HA  | 4        | 1.01          |
| (1,873)  | 1:B:67:GLU:H     | 1:B:67:GLU:HG2  | 1        | 1.01          |
| (1,873)  | 1:B:67:GLU:H     | 1:B:67:GLU:HG3  | 1        | 1.01          |
| (1,813)  | 1:A:145:VAL:HA   | 1:A:135:SER:H   | 6        | 1.01          |
| (1,69)   | 1:A:76:SER:HB3   | 1:A:146:ASP:HA  | 4        | 1.01          |
| (1,6)    | 1:A:67:GLU:H     | 1:A:67:GLU:HG2  | 1        | 1.01          |
| (1,6)    | 1:A:67:GLU:H     | 1:A:67:GLU:HG3  | 1        | 1.01          |
| (1,589)  | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG21 | 1        | 1.01          |
| (1,589)  | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG22 | 1        | 1.01          |
| (1,589)  | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG23 | 1        | 1.01          |
| (1,589)  | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG21 | 1        | 1.01          |
| (1,589)  | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG22 | 1        | 1.01          |
| (1,589)  | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG23 | 1        | 1.01          |
| (1,386)  | 1:A:102:GLY:HA2  | 1:A:102:GLY:HA3 | 1        | 1.01          |
| (1,381)  | 1:A:101:HIS:HA   | 1:A:102:GLY:H   | 2        | 1.01          |
| (1,199)  | 1:A:84:PHE:HB2   | 1:A:85:SER:H    | 1        | 1.01          |
| (1,199)  | 1:A:84:PHE:HB3   | 1:A:85:SER:H    | 1        | 1.01          |
| (1,199)  | 1:A:84:PHE:HB2   | 1:A:85:SER:H    | 5        | 1.01          |
| (1,199)  | 1:A:84:PHE:HB3   | 1:A:85:SER:H    | 5        | 1.01          |
| (1,1680) | 1:B:145:VAL:HA   | 1:B:135:SER:H   | 6        | 1.01          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG21 | 1        | 1.01          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG22 | 1        | 1.01          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG23 | 1        | 1.01          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG21 | 1        | 1.01          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG22 | 1        | 1.01          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG23 | 1        | 1.01          |
| (1,1253) | 1:B:102:GLY:HA2  | 1:B:102:GLY:HA3 | 1        | 1.01          |
| (1,1253) | 1:B:102:GLY:HA2  | 1:B:102:GLY:HA3 | 5        | 1.01          |
| (1,1248) | 1:B:101:HIS:HA   | 1:B:102:GLY:H   | 2        | 1.01          |
| (1,1066) | 1:B:84:PHE:HB2   | 1:B:85:SER:H    | 1        | 1.01          |
| (1,1066) | 1:B:84:PHE:HB3   | 1:B:85:SER:H    | 1        | 1.01          |
| (1,1066) | 1:B:84:PHE:HB2   | 1:B:85:SER:H    | 5        | 1.01          |
| (1,1066) | 1:B:84:PHE:HB3   | 1:B:85:SER:H    | 5        | 1.01          |
| (1,954)  | 1:B:77:VAL:HG21  | 1:B:75:PHE:HD1  | 4        | 1.0           |
| (1,954)  | 1:B:77:VAL:HG21  | 1:B:75:PHE:HD2  | 4        | 1.0           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,954)  | 1:B:77:VAL:HG22  | 1:B:75:PHE:HD1   | 4        | 1.0           |
| (1,954)  | 1:B:77:VAL:HG22  | 1:B:75:PHE:HD2   | 4        | 1.0           |
| (1,954)  | 1:B:77:VAL:HG23  | 1:B:75:PHE:HD1   | 4        | 1.0           |
| (1,954)  | 1:B:77:VAL:HG23  | 1:B:75:PHE:HD2   | 4        | 1.0           |
| (1,943)  | 1:B:76:SER:HB3   | 1:B:146:ASP:HA   | 7        | 1.0           |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD11  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD12  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD13  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD21  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD22  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD23  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD11  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD12  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD13  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD21  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD22  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD23  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD11  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD12  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD13  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD21  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD22  | 1        | 1.0           |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD23  | 1        | 1.0           |
| (1,76)   | 1:A:76:SER:HB3   | 1:A:146:ASP:HA   | 7        | 1.0           |
| (1,758)  | 1:A:138:SER:HA   | 1:A:141:GLY:H    | 8        | 1.0           |
| (1,739)  | 1:A:135:SER:HB3  | 1:A:145:VAL:HA   | 8        | 1.0           |
| (1,728)  | 1:A:133:ILE:HG12 | 1:A:147:GLY:HA2  | 3        | 1.0           |
| (1,728)  | 1:A:133:ILE:HG13 | 1:A:147:GLY:HA2  | 3        | 1.0           |
| (1,681)  | 1:A:128:VAL:H    | 1:A:150:LYS:HD2  | 7        | 1.0           |
| (1,681)  | 1:A:128:VAL:H    | 1:A:150:LYS:HD3  | 7        | 1.0           |
| (1,490)  | 1:A:113:PHE:HD1  | 1:A:113:PHE:HB2  | 3        | 1.0           |
| (1,490)  | 1:A:113:PHE:HD2  | 1:A:113:PHE:HB2  | 3        | 1.0           |
| (1,490)  | 1:A:113:PHE:HD1  | 1:A:113:PHE:HB2  | 9        | 1.0           |
| (1,490)  | 1:A:113:PHE:HD2  | 1:A:113:PHE:HB2  | 9        | 1.0           |
| (1,386)  | 1:A:102:GLY:HA2  | 1:A:102:GLY:HA3  | 5        | 1.0           |
| (1,386)  | 1:A:102:GLY:HA2  | 1:A:102:GLY:HA3  | 6        | 1.0           |
| (1,386)  | 1:A:102:GLY:HA2  | 1:A:102:GLY:HA3  | 8        | 1.0           |
| (1,386)  | 1:A:102:GLY:HA2  | 1:A:102:GLY:HA3  | 9        | 1.0           |
| (1,385)  | 1:A:102:GLY:HA2  | 1:A:84:PHE:HZ    | 8        | 1.0           |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG2   | 4        | 1.0           |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG3   | 4        | 1.0           |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG12 | 3        | 1.0           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG13 | 3        | 1.0           |
| (1,1625) | 1:B:138:SER:HA   | 1:B:141:GLY:H    | 8        | 1.0           |
| (1,1606) | 1:B:135:SER:HB3  | 1:B:145:VAL:HA   | 8        | 1.0           |
| (1,1595) | 1:B:133:ILE:HG12 | 1:B:147:GLY:HA2  | 3        | 1.0           |
| (1,1595) | 1:B:133:ILE:HG13 | 1:B:147:GLY:HA2  | 3        | 1.0           |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD2  | 7        | 1.0           |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD3  | 7        | 1.0           |
| (1,1357) | 1:B:113:PHE:HD1  | 1:B:113:PHE:HB2  | 3        | 1.0           |
| (1,1357) | 1:B:113:PHE:HD2  | 1:B:113:PHE:HB2  | 3        | 1.0           |
| (1,1357) | 1:B:113:PHE:HD1  | 1:B:113:PHE:HB2  | 9        | 1.0           |
| (1,1357) | 1:B:113:PHE:HD2  | 1:B:113:PHE:HB2  | 9        | 1.0           |
| (1,1253) | 1:B:102:GLY:HA2  | 1:B:102:GLY:HA3  | 6        | 1.0           |
| (1,1253) | 1:B:102:GLY:HA2  | 1:B:102:GLY:HA3  | 8        | 1.0           |
| (1,1253) | 1:B:102:GLY:HA2  | 1:B:102:GLY:HA3  | 9        | 1.0           |
| (1,1252) | 1:B:102:GLY:HA2  | 1:B:84:PHE:HZ    | 8        | 1.0           |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD11  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD12  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD13  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD21  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD22  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD23  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD11  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD12  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD13  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD21  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD22  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD23  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD11  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD12  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD13  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD21  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD22  | 1        | 1.0           |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD23  | 1        | 1.0           |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG2   | 4        | 1.0           |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG3   | 4        | 1.0           |
| (1,950)  | 1:B:77:VAL:HG11  | 1:B:68:MET:HA    | 1        | 0.99          |
| (1,950)  | 1:B:77:VAL:HG12  | 1:B:68:MET:HA    | 1        | 0.99          |
| (1,950)  | 1:B:77:VAL:HG13  | 1:B:68:MET:HA    | 1        | 0.99          |
| (1,873)  | 1:B:67:GLU:H     | 1:B:67:GLU:HG2   | 2        | 0.99          |
| (1,873)  | 1:B:67:GLU:H     | 1:B:67:GLU:HG3   | 2        | 0.99          |
| (1,873)  | 1:B:67:GLU:H     | 1:B:67:GLU:HG2   | 3        | 0.99          |
| (1,873)  | 1:B:67:GLU:H     | 1:B:67:GLU:HG3   | 3        | 0.99          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,873)  | 1:B:67:GLU:H     | 1:B:67:GLU:HG2  | 8        | 0.99          |
| (1,873)  | 1:B:67:GLU:H     | 1:B:67:GLU:HG3  | 8        | 0.99          |
| (1,87)   | 1:A:77:VAL:HG21  | 1:A:75:PHE:HD1  | 4        | 0.99          |
| (1,87)   | 1:A:77:VAL:HG21  | 1:A:75:PHE:HD2  | 4        | 0.99          |
| (1,87)   | 1:A:77:VAL:HG22  | 1:A:75:PHE:HD1  | 4        | 0.99          |
| (1,87)   | 1:A:77:VAL:HG22  | 1:A:75:PHE:HD2  | 4        | 0.99          |
| (1,87)   | 1:A:77:VAL:HG23  | 1:A:75:PHE:HD1  | 4        | 0.99          |
| (1,87)   | 1:A:77:VAL:HG23  | 1:A:75:PHE:HD2  | 4        | 0.99          |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE1  | 9        | 0.99          |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE2  | 9        | 0.99          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE1  | 9        | 0.99          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE2  | 9        | 0.99          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE1  | 9        | 0.99          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE2  | 9        | 0.99          |
| (1,6)    | 1:A:67:GLU:H     | 1:A:67:GLU:HG2  | 2        | 0.99          |
| (1,6)    | 1:A:67:GLU:H     | 1:A:67:GLU:HG3  | 2        | 0.99          |
| (1,6)    | 1:A:67:GLU:H     | 1:A:67:GLU:HG2  | 3        | 0.99          |
| (1,6)    | 1:A:67:GLU:H     | 1:A:67:GLU:HG3  | 3        | 0.99          |
| (1,6)    | 1:A:67:GLU:H     | 1:A:67:GLU:HG2  | 8        | 0.99          |
| (1,6)    | 1:A:67:GLU:H     | 1:A:67:GLU:HG3  | 8        | 0.99          |
| (1,598)  | 1:A:122:TYR:HB2  | 1:A:122:TYR:H   | 4        | 0.99          |
| (1,598)  | 1:A:122:TYR:HB3  | 1:A:122:TYR:H   | 4        | 0.99          |
| (1,597)  | 1:A:122:TYR:HB2  | 1:A:122:TYR:H   | 4        | 0.99          |
| (1,597)  | 1:A:122:TYR:HB3  | 1:A:122:TYR:H   | 4        | 0.99          |
| (1,497)  | 1:A:113:PHE:HD1  | 1:A:113:PHE:H   | 1        | 0.99          |
| (1,497)  | 1:A:113:PHE:HD2  | 1:A:113:PHE:H   | 1        | 0.99          |
| (1,397)  | 1:A:103:LYS:HG2  | 1:A:116:ARG:H   | 4        | 0.99          |
| (1,397)  | 1:A:103:LYS:HG3  | 1:A:116:ARG:H   | 4        | 0.99          |
| (1,386)  | 1:A:102:GLY:HA2  | 1:A:102:GLY:HA3 | 2        | 0.99          |
| (1,386)  | 1:A:102:GLY:HA2  | 1:A:102:GLY:HA3 | 4        | 0.99          |
| (1,386)  | 1:A:102:GLY:HA2  | 1:A:102:GLY:HA3 | 7        | 0.99          |
| (1,368)  | 1:A:101:HIS:HB2  | 1:A:92:LYS:HB2  | 8        | 0.99          |
| (1,368)  | 1:A:101:HIS:HB2  | 1:A:92:LYS:HB3  | 8        | 0.99          |
| (1,194)  | 1:A:84:PHE:HD1   | 1:A:83:HIS:H    | 1        | 0.99          |
| (1,194)  | 1:A:84:PHE:HD2   | 1:A:83:HIS:H    | 1        | 0.99          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE1  | 9        | 0.99          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE2  | 9        | 0.99          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE1  | 9        | 0.99          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE2  | 9        | 0.99          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE1  | 9        | 0.99          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE2  | 9        | 0.99          |
| (1,1465) | 1:B:122:TYR:HB2  | 1:B:122:TYR:H   | 4        | 0.99          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1465) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H    | 4        | 0.99          |
| (1,1464) | 1:B:122:TYR:HB2 | 1:B:122:TYR:H    | 4        | 0.99          |
| (1,1464) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H    | 4        | 0.99          |
| (1,1364) | 1:B:113:PHE:HD1 | 1:B:113:PHE:H    | 1        | 0.99          |
| (1,1364) | 1:B:113:PHE:HD2 | 1:B:113:PHE:H    | 1        | 0.99          |
| (1,1264) | 1:B:103:LYS:HG2 | 1:B:116:ARG:H    | 4        | 0.99          |
| (1,1264) | 1:B:103:LYS:HG3 | 1:B:116:ARG:H    | 4        | 0.99          |
| (1,1253) | 1:B:102:GLY:HA2 | 1:B:102:GLY:HA3  | 2        | 0.99          |
| (1,1253) | 1:B:102:GLY:HA2 | 1:B:102:GLY:HA3  | 4        | 0.99          |
| (1,1253) | 1:B:102:GLY:HA2 | 1:B:102:GLY:HA3  | 7        | 0.99          |
| (1,1235) | 1:B:101:HIS:HB2 | 1:B:92:LYS:HB2   | 8        | 0.99          |
| (1,1235) | 1:B:101:HIS:HB2 | 1:B:92:LYS:HB3   | 8        | 0.99          |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG11 | 2        | 0.99          |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG12 | 2        | 0.99          |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG13 | 2        | 0.99          |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG11 | 2        | 0.99          |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG12 | 2        | 0.99          |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG13 | 2        | 0.99          |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG11 | 2        | 0.99          |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG12 | 2        | 0.99          |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG13 | 2        | 0.99          |
| (1,1061) | 1:B:84:PHE:HD1  | 1:B:83:HIS:H     | 1        | 0.99          |
| (1,1061) | 1:B:84:PHE:HD2  | 1:B:83:HIS:H     | 1        | 0.99          |
| (1,83)   | 1:A:77:VAL:HG11 | 1:A:68:MET:HA    | 1        | 0.98          |
| (1,83)   | 1:A:77:VAL:HG12 | 1:A:68:MET:HA    | 1        | 0.98          |
| (1,83)   | 1:A:77:VAL:HG13 | 1:A:68:MET:HA    | 1        | 0.98          |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG21 | 7        | 0.98          |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG22 | 7        | 0.98          |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG23 | 7        | 0.98          |
| (1,603)  | 1:A:122:TYR:HA  | 1:A:124:ILE:HD11 | 4        | 0.98          |
| (1,603)  | 1:A:122:TYR:HA  | 1:A:124:ILE:HD12 | 4        | 0.98          |
| (1,603)  | 1:A:122:TYR:HA  | 1:A:124:ILE:HD13 | 4        | 0.98          |
| (1,570)  | 1:A:119:HIS:HA  | 1:A:101:HIS:HB3  | 2        | 0.98          |
| (1,440)  | 1:A:107:ARG:HB2 | 1:A:114:ILE:HG21 | 3        | 0.98          |
| (1,440)  | 1:A:107:ARG:HB2 | 1:A:114:ILE:HG22 | 3        | 0.98          |
| (1,440)  | 1:A:107:ARG:HB2 | 1:A:114:ILE:HG23 | 3        | 0.98          |
| (1,386)  | 1:A:102:GLY:HA2 | 1:A:102:GLY:HA3  | 3        | 0.98          |
| (1,321)  | 1:A:97:VAL:H    | 1:A:93:VAL:HB    | 4        | 0.98          |
| (1,268)  | 1:A:91:VAL:H    | 1:A:91:VAL:HG21  | 7        | 0.98          |
| (1,268)  | 1:A:91:VAL:H    | 1:A:91:VAL:HG22  | 7        | 0.98          |
| (1,268)  | 1:A:91:VAL:H    | 1:A:91:VAL:HG23  | 7        | 0.98          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG21 | 7        | 0.98          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG22 | 7        | 0.98          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG23 | 7        | 0.98          |
| (1,1470) | 1:B:122:TYR:HA  | 1:B:124:ILE:HD11 | 4        | 0.98          |
| (1,1470) | 1:B:122:TYR:HA  | 1:B:124:ILE:HD12 | 4        | 0.98          |
| (1,1470) | 1:B:122:TYR:HA  | 1:B:124:ILE:HD13 | 4        | 0.98          |
| (1,1437) | 1:B:119:HIS:HA  | 1:B:101:HIS:HB3  | 2        | 0.98          |
| (1,1307) | 1:B:107:ARG:HB2 | 1:B:114:ILE:HG21 | 3        | 0.98          |
| (1,1307) | 1:B:107:ARG:HB2 | 1:B:114:ILE:HG22 | 3        | 0.98          |
| (1,1307) | 1:B:107:ARG:HB2 | 1:B:114:ILE:HG23 | 3        | 0.98          |
| (1,1253) | 1:B:102:GLY:HA2 | 1:B:102:GLY:HA3  | 3        | 0.98          |
| (1,1188) | 1:B:97:VAL:H    | 1:B:93:VAL:HB    | 4        | 0.98          |
| (1,1135) | 1:B:91:VAL:H    | 1:B:91:VAL:HG21  | 7        | 0.98          |
| (1,1135) | 1:B:91:VAL:H    | 1:B:91:VAL:HG22  | 7        | 0.98          |
| (1,1135) | 1:B:91:VAL:H    | 1:B:91:VAL:HG23  | 7        | 0.98          |
| (1,97)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:H     | 4        | 0.97          |
| (1,97)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:H     | 4        | 0.97          |
| (1,97)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:H     | 4        | 0.97          |
| (1,964)  | 1:B:77:VAL:HG21 | 1:B:77:VAL:H     | 4        | 0.97          |
| (1,964)  | 1:B:77:VAL:HG22 | 1:B:77:VAL:H     | 4        | 0.97          |
| (1,964)  | 1:B:77:VAL:HG23 | 1:B:77:VAL:H     | 4        | 0.97          |
| (1,953)  | 1:B:77:VAL:HG21 | 1:B:75:PHE:HZ    | 3        | 0.97          |
| (1,953)  | 1:B:77:VAL:HG22 | 1:B:75:PHE:HZ    | 3        | 0.97          |
| (1,953)  | 1:B:77:VAL:HG23 | 1:B:75:PHE:HZ    | 3        | 0.97          |
| (1,598)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:H    | 2        | 0.97          |
| (1,598)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:H    | 2        | 0.97          |
| (1,597)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:H    | 2        | 0.97          |
| (1,597)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:H    | 2        | 0.97          |
| (1,568)  | 1:A:119:HIS:HB3 | 1:A:101:HIS:HA   | 7        | 0.97          |
| (1,497)  | 1:A:113:PHE:HD1 | 1:A:113:PHE:H    | 4        | 0.97          |
| (1,497)  | 1:A:113:PHE:HD2 | 1:A:113:PHE:H    | 4        | 0.97          |
| (1,490)  | 1:A:113:PHE:HD1 | 1:A:113:PHE:HB2  | 1        | 0.97          |
| (1,490)  | 1:A:113:PHE:HD2 | 1:A:113:PHE:HB2  | 1        | 0.97          |
| (1,342)  | 1:A:98:ILE:HD11 | 1:A:122:TYR:HD1  | 1        | 0.97          |
| (1,342)  | 1:A:98:ILE:HD11 | 1:A:122:TYR:HD2  | 1        | 0.97          |
| (1,342)  | 1:A:98:ILE:HD12 | 1:A:122:TYR:HD1  | 1        | 0.97          |
| (1,342)  | 1:A:98:ILE:HD12 | 1:A:122:TYR:HD2  | 1        | 0.97          |
| (1,342)  | 1:A:98:ILE:HD13 | 1:A:122:TYR:HD1  | 1        | 0.97          |
| (1,342)  | 1:A:98:ILE:HD13 | 1:A:122:TYR:HD2  | 1        | 0.97          |
| (1,236)  | 1:A:89:LEU:HD21 | 1:A:85:SER:HB3   | 7        | 0.97          |
| (1,236)  | 1:A:89:LEU:HD22 | 1:A:85:SER:HB3   | 7        | 0.97          |
| (1,236)  | 1:A:89:LEU:HD23 | 1:A:85:SER:HB3   | 7        | 0.97          |
| (1,1767) | 1:A:122:TYR:HB2 | 1:B:112:GLY:HA3  | 8        | 0.97          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1767) | 1:A:122:TYR:HB3 | 1:B:112:GLY:HA3 | 8        | 0.97          |
| (1,1472) | 1:B:123:ARG:HD2 | 1:B:98:ILE:H    | 3        | 0.97          |
| (1,1472) | 1:B:123:ARG:HD3 | 1:B:98:ILE:H    | 3        | 0.97          |
| (1,1465) | 1:B:122:TYR:HB2 | 1:B:122:TYR:H   | 2        | 0.97          |
| (1,1465) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H   | 2        | 0.97          |
| (1,1464) | 1:B:122:TYR:HB2 | 1:B:122:TYR:H   | 2        | 0.97          |
| (1,1464) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H   | 2        | 0.97          |
| (1,1435) | 1:B:119:HIS:HB3 | 1:B:101:HIS:HA  | 7        | 0.97          |
| (1,140)  | 1:A:79:LEU:HD11 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,140)  | 1:A:79:LEU:HD12 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,140)  | 1:A:79:LEU:HD13 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,140)  | 1:A:79:LEU:HD21 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,140)  | 1:A:79:LEU:HD22 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,140)  | 1:A:79:LEU:HD23 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,139)  | 1:A:79:LEU:HD11 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,139)  | 1:A:79:LEU:HD12 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,139)  | 1:A:79:LEU:HD13 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,139)  | 1:A:79:LEU:HD21 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,139)  | 1:A:79:LEU:HD22 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,139)  | 1:A:79:LEU:HD23 | 1:A:79:LEU:H    | 9        | 0.97          |
| (1,1357) | 1:B:113:PHE:HD1 | 1:B:113:PHE:HB2 | 1        | 0.97          |
| (1,1357) | 1:B:113:PHE:HD2 | 1:B:113:PHE:HB2 | 1        | 0.97          |
| (1,1324) | 1:B:111:HIS:H   | 1:B:109:ASP:HB2 | 5        | 0.97          |
| (1,1324) | 1:B:111:HIS:H   | 1:B:109:ASP:HB3 | 5        | 0.97          |
| (1,1209) | 1:B:98:ILE:HD11 | 1:B:122:TYR:HD1 | 1        | 0.97          |
| (1,1209) | 1:B:98:ILE:HD11 | 1:B:122:TYR:HD2 | 1        | 0.97          |
| (1,1209) | 1:B:98:ILE:HD12 | 1:B:122:TYR:HD1 | 1        | 0.97          |
| (1,1209) | 1:B:98:ILE:HD12 | 1:B:122:TYR:HD2 | 1        | 0.97          |
| (1,1209) | 1:B:98:ILE:HD13 | 1:B:122:TYR:HD1 | 1        | 0.97          |
| (1,1209) | 1:B:98:ILE:HD13 | 1:B:122:TYR:HD2 | 1        | 0.97          |
| (1,1103) | 1:B:89:LEU:HD21 | 1:B:85:SER:HB3  | 7        | 0.97          |
| (1,1103) | 1:B:89:LEU:HD22 | 1:B:85:SER:HB3  | 7        | 0.97          |
| (1,1103) | 1:B:89:LEU:HD23 | 1:B:85:SER:HB3  | 7        | 0.97          |
| (1,1007) | 1:B:79:LEU:HD11 | 1:B:79:LEU:H    | 9        | 0.97          |
| (1,1007) | 1:B:79:LEU:HD12 | 1:B:79:LEU:H    | 9        | 0.97          |
| (1,1007) | 1:B:79:LEU:HD13 | 1:B:79:LEU:H    | 9        | 0.97          |
| (1,1007) | 1:B:79:LEU:HD21 | 1:B:79:LEU:H    | 9        | 0.97          |
| (1,1007) | 1:B:79:LEU:HD22 | 1:B:79:LEU:H    | 9        | 0.97          |
| (1,1007) | 1:B:79:LEU:HD23 | 1:B:79:LEU:H    | 9        | 0.97          |
| (1,1006) | 1:B:79:LEU:HD11 | 1:B:79:LEU:H    | 9        | 0.97          |
| (1,1006) | 1:B:79:LEU:HD12 | 1:B:79:LEU:H    | 9        | 0.97          |
| (1,1006) | 1:B:79:LEU:HD13 | 1:B:79:LEU:H    | 9        | 0.97          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1006) | 1:B:79:LEU:HD21 | 1:B:79:LEU:H     | 9        | 0.97          |
| (1,1006) | 1:B:79:LEU:HD22 | 1:B:79:LEU:H     | 9        | 0.97          |
| (1,1006) | 1:B:79:LEU:HD23 | 1:B:79:LEU:H     | 9        | 0.97          |
| (1,964)  | 1:B:77:VAL:HG21 | 1:B:77:VAL:H     | 8        | 0.96          |
| (1,964)  | 1:B:77:VAL:HG22 | 1:B:77:VAL:H     | 8        | 0.96          |
| (1,964)  | 1:B:77:VAL:HG23 | 1:B:77:VAL:H     | 8        | 0.96          |
| (1,739)  | 1:A:135:SER:HB3 | 1:A:145:VAL:HA   | 9        | 0.96          |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG21 | 5        | 0.96          |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG22 | 5        | 0.96          |
| (1,649)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HG23 | 5        | 0.96          |
| (1,605)  | 1:A:123:ARG:HD2 | 1:A:98:ILE:H     | 3        | 0.96          |
| (1,605)  | 1:A:123:ARG:HD3 | 1:A:98:ILE:H     | 3        | 0.96          |
| (1,457)  | 1:A:111:HIS:H   | 1:A:109:ASP:HB2  | 5        | 0.96          |
| (1,457)  | 1:A:111:HIS:H   | 1:A:109:ASP:HB3  | 5        | 0.96          |
| (1,258)  | 1:A:89:LEU:HD11 | 1:A:102:GLY:HA2  | 2        | 0.96          |
| (1,258)  | 1:A:89:LEU:HD12 | 1:A:102:GLY:HA2  | 2        | 0.96          |
| (1,258)  | 1:A:89:LEU:HD13 | 1:A:102:GLY:HA2  | 2        | 0.96          |
| (1,257)  | 1:A:89:LEU:HD11 | 1:A:102:GLY:HA2  | 2        | 0.96          |
| (1,257)  | 1:A:89:LEU:HD12 | 1:A:102:GLY:HA2  | 2        | 0.96          |
| (1,257)  | 1:A:89:LEU:HD13 | 1:A:102:GLY:HA2  | 2        | 0.96          |
| (1,217)  | 1:A:86:PRO:HB2  | 1:A:84:PHE:HD1   | 5        | 0.96          |
| (1,217)  | 1:A:86:PRO:HB2  | 1:A:84:PHE:HD2   | 5        | 0.96          |
| (1,217)  | 1:A:86:PRO:HB3  | 1:A:84:PHE:HD1   | 5        | 0.96          |
| (1,217)  | 1:A:86:PRO:HB3  | 1:A:84:PHE:HD2   | 5        | 0.96          |
| (1,210)  | 1:A:85:SER:HB2  | 1:A:87:GLU:HG2   | 8        | 0.96          |
| (1,210)  | 1:A:85:SER:HB2  | 1:A:87:GLU:HG3   | 8        | 0.96          |
| (1,1770) | 1:A:123:ARG:HD2 | 1:B:113:PHE:H    | 4        | 0.96          |
| (1,1770) | 1:A:123:ARG:HD3 | 1:B:113:PHE:H    | 4        | 0.96          |
| (1,1606) | 1:B:135:SER:HB3 | 1:B:145:VAL:HA   | 9        | 0.96          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG21 | 5        | 0.96          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG22 | 5        | 0.96          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG23 | 5        | 0.96          |
| (1,1364) | 1:B:113:PHE:HD1 | 1:B:113:PHE:H    | 4        | 0.96          |
| (1,1364) | 1:B:113:PHE:HD2 | 1:B:113:PHE:H    | 4        | 0.96          |
| (1,1125) | 1:B:89:LEU:HD11 | 1:B:102:GLY:HA2  | 2        | 0.96          |
| (1,1125) | 1:B:89:LEU:HD12 | 1:B:102:GLY:HA2  | 2        | 0.96          |
| (1,1125) | 1:B:89:LEU:HD13 | 1:B:102:GLY:HA2  | 2        | 0.96          |
| (1,1124) | 1:B:89:LEU:HD11 | 1:B:102:GLY:HA2  | 2        | 0.96          |
| (1,1124) | 1:B:89:LEU:HD12 | 1:B:102:GLY:HA2  | 2        | 0.96          |
| (1,1124) | 1:B:89:LEU:HD13 | 1:B:102:GLY:HA2  | 2        | 0.96          |
| (1,1084) | 1:B:86:PRO:HB2  | 1:B:84:PHE:HD1   | 5        | 0.96          |
| (1,1084) | 1:B:86:PRO:HB2  | 1:B:84:PHE:HD2   | 5        | 0.96          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1084) | 1:B:86:PRO:HB3  | 1:B:84:PHE:HD1  | 5        | 0.96          |
| (1,1084) | 1:B:86:PRO:HB3  | 1:B:84:PHE:HD2  | 5        | 0.96          |
| (1,1077) | 1:B:85:SER:HB2  | 1:B:87:GLU:HG2  | 8        | 0.96          |
| (1,1077) | 1:B:85:SER:HB2  | 1:B:87:GLU:HG3  | 8        | 0.96          |
| (1,993)  | 1:B:78:ASN:H    | 1:B:78:ASN:HD22 | 3        | 0.95          |
| (1,977)  | 1:B:77:VAL:HG11 | 1:B:98:ILE:HD11 | 4        | 0.95          |
| (1,977)  | 1:B:77:VAL:HG11 | 1:B:98:ILE:HD12 | 4        | 0.95          |
| (1,977)  | 1:B:77:VAL:HG11 | 1:B:98:ILE:HD13 | 4        | 0.95          |
| (1,977)  | 1:B:77:VAL:HG12 | 1:B:98:ILE:HD11 | 4        | 0.95          |
| (1,977)  | 1:B:77:VAL:HG12 | 1:B:98:ILE:HD12 | 4        | 0.95          |
| (1,977)  | 1:B:77:VAL:HG12 | 1:B:98:ILE:HD13 | 4        | 0.95          |
| (1,977)  | 1:B:77:VAL:HG13 | 1:B:98:ILE:HD11 | 4        | 0.95          |
| (1,977)  | 1:B:77:VAL:HG13 | 1:B:98:ILE:HD12 | 4        | 0.95          |
| (1,977)  | 1:B:77:VAL:HG13 | 1:B:98:ILE:HD13 | 4        | 0.95          |
| (1,97)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:H    | 8        | 0.95          |
| (1,97)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:H    | 8        | 0.95          |
| (1,97)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:H    | 8        | 0.95          |
| (1,963)  | 1:B:77:VAL:HG21 | 1:B:77:VAL:HB   | 1        | 0.95          |
| (1,963)  | 1:B:77:VAL:HG22 | 1:B:77:VAL:HB   | 1        | 0.95          |
| (1,963)  | 1:B:77:VAL:HG23 | 1:B:77:VAL:HB   | 1        | 0.95          |
| (1,96)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:HB   | 1        | 0.95          |
| (1,96)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:HB   | 1        | 0.95          |
| (1,96)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:HB   | 1        | 0.95          |
| (1,953)  | 1:B:77:VAL:HG21 | 1:B:75:PHE:HZ   | 2        | 0.95          |
| (1,953)  | 1:B:77:VAL:HG22 | 1:B:75:PHE:HZ   | 2        | 0.95          |
| (1,953)  | 1:B:77:VAL:HG23 | 1:B:75:PHE:HZ   | 2        | 0.95          |
| (1,936)  | 1:B:76:SER:HB3  | 1:B:146:ASP:HA  | 7        | 0.95          |
| (1,862)  | 1:A:150:LYS:HG2 | 1:A:151:GLN:H   | 4        | 0.95          |
| (1,862)  | 1:A:150:LYS:HG3 | 1:A:151:GLN:H   | 4        | 0.95          |
| (1,734)  | 1:A:135:SER:H   | 1:A:134:THR:HB  | 4        | 0.95          |
| (1,709)  | 1:A:132:THR:HB  | 1:A:147:GLY:HA3 | 8        | 0.95          |
| (1,69)   | 1:A:76:SER:HB3  | 1:A:146:ASP:HA  | 7        | 0.95          |
| (1,598)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:H   | 3        | 0.95          |
| (1,598)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:H   | 3        | 0.95          |
| (1,597)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:H   | 3        | 0.95          |
| (1,597)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:H   | 3        | 0.95          |
| (1,568)  | 1:A:119:HIS:HB3 | 1:A:101:HIS:HA  | 1        | 0.95          |
| (1,490)  | 1:A:113:PHE:HD1 | 1:A:113:PHE:HB2 | 4        | 0.95          |
| (1,490)  | 1:A:113:PHE:HD2 | 1:A:113:PHE:HB2 | 4        | 0.95          |
| (1,381)  | 1:A:101:HIS:HA  | 1:A:102:GLY:H   | 7        | 0.95          |
| (1,1729) | 1:B:150:LYS:HG2 | 1:B:151:GLN:H   | 4        | 0.95          |
| (1,1729) | 1:B:150:LYS:HG3 | 1:B:151:GLN:H   | 4        | 0.95          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1601) | 1:B:135:SER:H    | 1:B:134:THR:HB  | 4        | 0.95          |
| (1,1576) | 1:B:132:THR:HB   | 1:B:147:GLY:HA3 | 8        | 0.95          |
| (1,1465) | 1:B:122:TYR:HB2  | 1:B:122:TYR:H   | 3        | 0.95          |
| (1,1465) | 1:B:122:TYR:HB3  | 1:B:122:TYR:H   | 3        | 0.95          |
| (1,1464) | 1:B:122:TYR:HB2  | 1:B:122:TYR:H   | 3        | 0.95          |
| (1,1464) | 1:B:122:TYR:HB3  | 1:B:122:TYR:H   | 3        | 0.95          |
| (1,1435) | 1:B:119:HIS:HB3  | 1:B:101:HIS:HA  | 1        | 0.95          |
| (1,1357) | 1:B:113:PHE:HD1  | 1:B:113:PHE:HB2 | 4        | 0.95          |
| (1,1357) | 1:B:113:PHE:HD2  | 1:B:113:PHE:HB2 | 4        | 0.95          |
| (1,126)  | 1:A:78:ASN:H     | 1:A:78:ASN:HD22 | 3        | 0.95          |
| (1,1248) | 1:B:101:HIS:HA   | 1:B:102:GLY:H   | 7        | 0.95          |
| (1,963)  | 1:B:77:VAL:HG21  | 1:B:77:VAL:HB   | 5        | 0.94          |
| (1,963)  | 1:B:77:VAL:HG22  | 1:B:77:VAL:HB   | 5        | 0.94          |
| (1,963)  | 1:B:77:VAL:HG23  | 1:B:77:VAL:HB   | 5        | 0.94          |
| (1,963)  | 1:B:77:VAL:HG21  | 1:B:77:VAL:HB   | 7        | 0.94          |
| (1,963)  | 1:B:77:VAL:HG22  | 1:B:77:VAL:HB   | 7        | 0.94          |
| (1,963)  | 1:B:77:VAL:HG23  | 1:B:77:VAL:HB   | 7        | 0.94          |
| (1,96)   | 1:A:77:VAL:HG21  | 1:A:77:VAL:HB   | 5        | 0.94          |
| (1,96)   | 1:A:77:VAL:HG22  | 1:A:77:VAL:HB   | 5        | 0.94          |
| (1,96)   | 1:A:77:VAL:HG23  | 1:A:77:VAL:HB   | 5        | 0.94          |
| (1,96)   | 1:A:77:VAL:HG21  | 1:A:77:VAL:HB   | 7        | 0.94          |
| (1,96)   | 1:A:77:VAL:HG22  | 1:A:77:VAL:HB   | 7        | 0.94          |
| (1,96)   | 1:A:77:VAL:HG23  | 1:A:77:VAL:HB   | 7        | 0.94          |
| (1,861)  | 1:A:150:LYS:HA   | 1:A:151:GLN:H   | 1        | 0.94          |
| (1,861)  | 1:A:150:LYS:HA   | 1:A:151:GLN:H   | 2        | 0.94          |
| (1,86)   | 1:A:77:VAL:HG21  | 1:A:75:PHE:HZ   | 3        | 0.94          |
| (1,86)   | 1:A:77:VAL:HG22  | 1:A:75:PHE:HZ   | 3        | 0.94          |
| (1,86)   | 1:A:77:VAL:HG23  | 1:A:75:PHE:HZ   | 3        | 0.94          |
| (1,859)  | 1:A:150:LYS:H    | 1:A:150:LYS:HG2 | 7        | 0.94          |
| (1,859)  | 1:A:150:LYS:H    | 1:A:150:LYS:HG3 | 7        | 0.94          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD2 | 6        | 0.94          |
| (1,849)  | 1:A:147:GLY:HA2  | 1:A:148:PRO:HD3 | 6        | 0.94          |
| (1,651)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HA  | 2        | 0.94          |
| (1,598)  | 1:A:122:TYR:HB2  | 1:A:122:TYR:H   | 8        | 0.94          |
| (1,598)  | 1:A:122:TYR:HB3  | 1:A:122:TYR:H   | 8        | 0.94          |
| (1,597)  | 1:A:122:TYR:HB2  | 1:A:122:TYR:H   | 8        | 0.94          |
| (1,597)  | 1:A:122:TYR:HB3  | 1:A:122:TYR:H   | 8        | 0.94          |
| (1,555)  | 1:A:118:PHE:HB2  | 1:A:117:GLU:H   | 9        | 0.94          |
| (1,539)  | 1:A:116:ARG:H    | 1:A:116:ARG:HG2 | 9        | 0.94          |
| (1,539)  | 1:A:116:ARG:H    | 1:A:116:ARG:HG3 | 9        | 0.94          |
| (1,507)  | 1:A:114:ILE:HD11 | 1:A:107:ARG:HD3 | 8        | 0.94          |
| (1,507)  | 1:A:114:ILE:HD12 | 1:A:107:ARG:HD3 | 8        | 0.94          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,507)  | 1:A:114:ILE:HD13 | 1:A:107:ARG:HD3 | 8        | 0.94          |
| (1,490)  | 1:A:113:PHE:HD1  | 1:A:113:PHE:HB2 | 6        | 0.94          |
| (1,490)  | 1:A:113:PHE:HD2  | 1:A:113:PHE:HB2 | 6        | 0.94          |
| (1,490)  | 1:A:113:PHE:HD1  | 1:A:113:PHE:HB2 | 8        | 0.94          |
| (1,490)  | 1:A:113:PHE:HD2  | 1:A:113:PHE:HB2 | 8        | 0.94          |
| (1,1728) | 1:B:150:LYS:HA   | 1:B:151:GLN:H   | 1        | 0.94          |
| (1,1728) | 1:B:150:LYS:HA   | 1:B:151:GLN:H   | 2        | 0.94          |
| (1,1726) | 1:B:150:LYS:H    | 1:B:150:LYS:HG2 | 7        | 0.94          |
| (1,1726) | 1:B:150:LYS:H    | 1:B:150:LYS:HG3 | 7        | 0.94          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD2 | 6        | 0.94          |
| (1,1716) | 1:B:147:GLY:HA2  | 1:B:148:PRO:HD3 | 6        | 0.94          |
| (1,160)  | 1:A:81:VAL:H     | 1:A:82:LYS:H    | 7        | 0.94          |
| (1,159)  | 1:A:81:VAL:H     | 1:A:82:LYS:H    | 7        | 0.94          |
| (1,1518) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HA  | 2        | 0.94          |
| (1,151)  | 1:A:81:VAL:HG11  | 1:A:79:LEU:HG   | 3        | 0.94          |
| (1,151)  | 1:A:81:VAL:HG12  | 1:A:79:LEU:HG   | 3        | 0.94          |
| (1,151)  | 1:A:81:VAL:HG13  | 1:A:79:LEU:HG   | 3        | 0.94          |
| (1,1465) | 1:B:122:TYR:HB2  | 1:B:122:TYR:H   | 8        | 0.94          |
| (1,1465) | 1:B:122:TYR:HB3  | 1:B:122:TYR:H   | 8        | 0.94          |
| (1,1464) | 1:B:122:TYR:HB2  | 1:B:122:TYR:H   | 8        | 0.94          |
| (1,1464) | 1:B:122:TYR:HB3  | 1:B:122:TYR:H   | 8        | 0.94          |
| (1,1422) | 1:B:118:PHE:HB2  | 1:B:117:GLU:H   | 9        | 0.94          |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG2 | 9        | 0.94          |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG3 | 9        | 0.94          |
| (1,140)  | 1:A:79:LEU:HD11  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,140)  | 1:A:79:LEU:HD12  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,140)  | 1:A:79:LEU:HD13  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,140)  | 1:A:79:LEU:HD21  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,140)  | 1:A:79:LEU:HD22  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,140)  | 1:A:79:LEU:HD23  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,139)  | 1:A:79:LEU:HD11  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,139)  | 1:A:79:LEU:HD12  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,139)  | 1:A:79:LEU:HD13  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,139)  | 1:A:79:LEU:HD21  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,139)  | 1:A:79:LEU:HD22  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,139)  | 1:A:79:LEU:HD23  | 1:A:79:LEU:H    | 5        | 0.94          |
| (1,1357) | 1:B:113:PHE:HD1  | 1:B:113:PHE:HB2 | 6        | 0.94          |
| (1,1357) | 1:B:113:PHE:HD2  | 1:B:113:PHE:HB2 | 6        | 0.94          |
| (1,1357) | 1:B:113:PHE:HD1  | 1:B:113:PHE:HB2 | 8        | 0.94          |
| (1,1357) | 1:B:113:PHE:HD2  | 1:B:113:PHE:HB2 | 8        | 0.94          |
| (1,1027) | 1:B:81:VAL:H     | 1:B:82:LYS:H    | 7        | 0.94          |
| (1,1026) | 1:B:81:VAL:H     | 1:B:82:LYS:H    | 7        | 0.94          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1018) | 1:B:81:VAL:HG11 | 1:B:79:LEU:HG   | 3        | 0.94          |
| (1,1018) | 1:B:81:VAL:HG12 | 1:B:79:LEU:HG   | 3        | 0.94          |
| (1,1018) | 1:B:81:VAL:HG13 | 1:B:79:LEU:HG   | 3        | 0.94          |
| (1,963)  | 1:B:77:VAL:HG21 | 1:B:77:VAL:HB   | 2        | 0.93          |
| (1,963)  | 1:B:77:VAL:HG22 | 1:B:77:VAL:HB   | 2        | 0.93          |
| (1,963)  | 1:B:77:VAL:HG23 | 1:B:77:VAL:HB   | 2        | 0.93          |
| (1,963)  | 1:B:77:VAL:HG21 | 1:B:77:VAL:HB   | 3        | 0.93          |
| (1,963)  | 1:B:77:VAL:HG22 | 1:B:77:VAL:HB   | 3        | 0.93          |
| (1,963)  | 1:B:77:VAL:HG23 | 1:B:77:VAL:HB   | 3        | 0.93          |
| (1,963)  | 1:B:77:VAL:HG21 | 1:B:77:VAL:HB   | 6        | 0.93          |
| (1,963)  | 1:B:77:VAL:HG22 | 1:B:77:VAL:HB   | 6        | 0.93          |
| (1,963)  | 1:B:77:VAL:HG23 | 1:B:77:VAL:HB   | 6        | 0.93          |
| (1,963)  | 1:B:77:VAL:HG21 | 1:B:77:VAL:HB   | 8        | 0.93          |
| (1,963)  | 1:B:77:VAL:HG22 | 1:B:77:VAL:HB   | 8        | 0.93          |
| (1,963)  | 1:B:77:VAL:HG23 | 1:B:77:VAL:HB   | 8        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:HB   | 2        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:HB   | 2        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:HB   | 2        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:HB   | 3        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:HB   | 3        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:HB   | 3        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:HB   | 4        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:HB   | 4        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:HB   | 4        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:HB   | 6        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:HB   | 6        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:HB   | 6        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:HB   | 8        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:HB   | 8        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:HB   | 8        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:HB   | 9        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:HB   | 9        | 0.93          |
| (1,96)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:HB   | 9        | 0.93          |
| (1,86)   | 1:A:77:VAL:HG21 | 1:A:75:PHE:HZ   | 2        | 0.93          |
| (1,86)   | 1:A:77:VAL:HG22 | 1:A:75:PHE:HZ   | 2        | 0.93          |
| (1,86)   | 1:A:77:VAL:HG23 | 1:A:75:PHE:HZ   | 2        | 0.93          |
| (1,841)  | 1:A:147:GLY:HA2 | 1:A:132:THR:HA  | 6        | 0.93          |
| (1,739)  | 1:A:135:SER:HB3 | 1:A:145:VAL:HA  | 7        | 0.93          |
| (1,686)  | 1:A:129:ASP:H   | 1:A:132:THR:HG1 | 8        | 0.93          |
| (1,600)  | 1:A:122:TYR:HA  | 1:A:123:ARG:HB3 | 3        | 0.93          |
| (1,490)  | 1:A:113:PHE:HD1 | 1:A:113:PHE:HB2 | 5        | 0.93          |
| (1,490)  | 1:A:113:PHE:HD2 | 1:A:113:PHE:HB2 | 5        | 0.93          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,481)  | 1:A:113:PHE:HA   | 1:A:107:ARG:HB2 | 3        | 0.93          |
| (1,403)  | 1:A:104:HIS:HA   | 1:A:104:HIS:HD2 | 1        | 0.93          |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG2 | 1        | 0.93          |
| (1,319)  | 1:A:96:ASP:H     | 1:A:123:ARG:HG3 | 1        | 0.93          |
| (1,1745) | 1:A:114:ILE:H    | 1:B:121:LYS:H   | 9        | 0.93          |
| (1,1732) | 1:B:151:GLN:H    | 1:B:151:GLN:HG2 | 4        | 0.93          |
| (1,1732) | 1:B:151:GLN:H    | 1:B:151:GLN:HG3 | 4        | 0.93          |
| (1,1710) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HB  | 5        | 0.93          |
| (1,1708) | 1:B:147:GLY:HA2  | 1:B:132:THR:HA  | 6        | 0.93          |
| (1,1606) | 1:B:135:SER:HB3  | 1:B:145:VAL:HA  | 7        | 0.93          |
| (1,1467) | 1:B:122:TYR:HA   | 1:B:123:ARG:HB3 | 3        | 0.93          |
| (1,1374) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HD3 | 8        | 0.93          |
| (1,1374) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HD3 | 8        | 0.93          |
| (1,1374) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HD3 | 8        | 0.93          |
| (1,1357) | 1:B:113:PHE:HD1  | 1:B:113:PHE:HB2 | 5        | 0.93          |
| (1,1357) | 1:B:113:PHE:HD2  | 1:B:113:PHE:HB2 | 5        | 0.93          |
| (1,1348) | 1:B:113:PHE:HA   | 1:B:107:ARG:HB2 | 3        | 0.93          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG2 | 1        | 0.93          |
| (1,1186) | 1:B:96:ASP:H     | 1:B:123:ARG:HG3 | 1        | 0.93          |
| (1,110)  | 1:A:77:VAL:HG11  | 1:A:98:ILE:HD11 | 4        | 0.93          |
| (1,110)  | 1:A:77:VAL:HG11  | 1:A:98:ILE:HD12 | 4        | 0.93          |
| (1,110)  | 1:A:77:VAL:HG11  | 1:A:98:ILE:HD13 | 4        | 0.93          |
| (1,110)  | 1:A:77:VAL:HG12  | 1:A:98:ILE:HD11 | 4        | 0.93          |
| (1,110)  | 1:A:77:VAL:HG12  | 1:A:98:ILE:HD12 | 4        | 0.93          |
| (1,110)  | 1:A:77:VAL:HG12  | 1:A:98:ILE:HD13 | 4        | 0.93          |
| (1,110)  | 1:A:77:VAL:HG13  | 1:A:98:ILE:HD11 | 4        | 0.93          |
| (1,110)  | 1:A:77:VAL:HG13  | 1:A:98:ILE:HD12 | 4        | 0.93          |
| (1,110)  | 1:A:77:VAL:HG13  | 1:A:98:ILE:HD13 | 4        | 0.93          |
| (1,1007) | 1:B:79:LEU:HD11  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,1007) | 1:B:79:LEU:HD12  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,1007) | 1:B:79:LEU:HD13  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,1007) | 1:B:79:LEU:HD21  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,1007) | 1:B:79:LEU:HD22  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,1007) | 1:B:79:LEU:HD23  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,1006) | 1:B:79:LEU:HD11  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,1006) | 1:B:79:LEU:HD12  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,1006) | 1:B:79:LEU:HD13  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,1006) | 1:B:79:LEU:HD21  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,1006) | 1:B:79:LEU:HD22  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,1006) | 1:B:79:LEU:HD23  | 1:B:79:LEU:H    | 5        | 0.93          |
| (1,993)  | 1:B:78:ASN:H     | 1:B:78:ASN:HD22 | 5        | 0.92          |
| (1,963)  | 1:B:77:VAL:HG21  | 1:B:77:VAL:HB   | 4        | 0.92          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,963)  | 1:B:77:VAL:HG22  | 1:B:77:VAL:HB   | 4        | 0.92          |
| (1,963)  | 1:B:77:VAL:HG23  | 1:B:77:VAL:HB   | 4        | 0.92          |
| (1,963)  | 1:B:77:VAL:HG21  | 1:B:77:VAL:HB   | 9        | 0.92          |
| (1,963)  | 1:B:77:VAL:HG22  | 1:B:77:VAL:HB   | 9        | 0.92          |
| (1,963)  | 1:B:77:VAL:HG23  | 1:B:77:VAL:HB   | 9        | 0.92          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD11 | 9        | 0.92          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD12 | 9        | 0.92          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD13 | 9        | 0.92          |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD11 | 9        | 0.92          |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD12 | 9        | 0.92          |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD13 | 9        | 0.92          |
| (1,865)  | 1:A:151:GLN:H    | 1:A:151:GLN:HG2 | 4        | 0.92          |
| (1,865)  | 1:A:151:GLN:H    | 1:A:151:GLN:HG3 | 4        | 0.92          |
| (1,861)  | 1:A:150:LYS:HA   | 1:A:151:GLN:H   | 3        | 0.92          |
| (1,843)  | 1:A:147:GLY:HA2  | 1:A:133:ILE:HB  | 5        | 0.92          |
| (1,571)  | 1:A:119:HIS:HA   | 1:A:101:HIS:HD2 | 2        | 0.92          |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB2 | 9        | 0.92          |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB3 | 9        | 0.92          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD11 | 9        | 0.92          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD12 | 9        | 0.92          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD13 | 9        | 0.92          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD11 | 9        | 0.92          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD12 | 9        | 0.92          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD13 | 9        | 0.92          |
| (1,518)  | 1:A:114:ILE:HG21 | 1:A:114:ILE:H   | 3        | 0.92          |
| (1,518)  | 1:A:114:ILE:HG22 | 1:A:114:ILE:H   | 3        | 0.92          |
| (1,518)  | 1:A:114:ILE:HG23 | 1:A:114:ILE:H   | 3        | 0.92          |
| (1,403)  | 1:A:104:HIS:HA   | 1:A:104:HIS:HD2 | 6        | 0.92          |
| (1,1749) | 1:A:115:SER:HB3  | 1:B:119:HIS:HE1 | 4        | 0.92          |
| (1,1740) | 1:A:113:PHE:HD1  | 1:B:121:LYS:H   | 3        | 0.92          |
| (1,1740) | 1:A:113:PHE:HD2  | 1:B:121:LYS:H   | 3        | 0.92          |
| (1,1728) | 1:B:150:LYS:HA   | 1:B:151:GLN:H   | 3        | 0.92          |
| (1,1438) | 1:B:119:HIS:HA   | 1:B:101:HIS:HD2 | 2        | 0.92          |
| (1,1385) | 1:B:114:ILE:HG21 | 1:B:114:ILE:H   | 3        | 0.92          |
| (1,1385) | 1:B:114:ILE:HG22 | 1:B:114:ILE:H   | 3        | 0.92          |
| (1,1385) | 1:B:114:ILE:HG23 | 1:B:114:ILE:H   | 3        | 0.92          |
| (1,1270) | 1:B:104:HIS:HA   | 1:B:104:HIS:HD2 | 2        | 0.92          |
| (1,1270) | 1:B:104:HIS:HA   | 1:B:104:HIS:HD2 | 6        | 0.92          |
| (1,126)  | 1:A:78:ASN:H     | 1:A:78:ASN:HD22 | 5        | 0.92          |
| (1,993)  | 1:B:78:ASN:H     | 1:B:78:ASN:HD22 | 4        | 0.91          |
| (1,953)  | 1:B:77:VAL:HG21  | 1:B:75:PHE:HZ   | 5        | 0.91          |
| (1,953)  | 1:B:77:VAL:HG22  | 1:B:75:PHE:HZ   | 5        | 0.91          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,953)  | 1:B:77:VAL:HG23  | 1:B:75:PHE:HZ    | 5        | 0.91          |
| (1,862)  | 1:A:150:LYS:HG2  | 1:A:151:GLN:H    | 3        | 0.91          |
| (1,862)  | 1:A:150:LYS:HG3  | 1:A:151:GLN:H    | 3        | 0.91          |
| (1,86)   | 1:A:77:VAL:HG21  | 1:A:75:PHE:HZ    | 5        | 0.91          |
| (1,86)   | 1:A:77:VAL:HG22  | 1:A:75:PHE:HZ    | 5        | 0.91          |
| (1,86)   | 1:A:77:VAL:HG23  | 1:A:75:PHE:HZ    | 5        | 0.91          |
| (1,841)  | 1:A:147:GLY:HA2  | 1:A:132:THR:HA   | 4        | 0.91          |
| (1,651)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HA   | 5        | 0.91          |
| (1,563)  | 1:A:118:PHE:HB2  | 1:A:118:PHE:H    | 3        | 0.91          |
| (1,513)  | 1:A:114:ILE:HA   | 1:A:114:ILE:HB   | 3        | 0.91          |
| (1,504)  | 1:A:114:ILE:HD11 | 1:A:107:ARG:HD2  | 8        | 0.91          |
| (1,504)  | 1:A:114:ILE:HD12 | 1:A:107:ARG:HD2  | 8        | 0.91          |
| (1,504)  | 1:A:114:ILE:HD13 | 1:A:107:ARG:HD2  | 8        | 0.91          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG21  | 3        | 0.91          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG22  | 3        | 0.91          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG23  | 3        | 0.91          |
| (1,1745) | 1:A:114:ILE:H    | 1:B:121:LYS:H    | 5        | 0.91          |
| (1,1729) | 1:B:150:LYS:HG2  | 1:B:151:GLN:H    | 3        | 0.91          |
| (1,1729) | 1:B:150:LYS:HG3  | 1:B:151:GLN:H    | 3        | 0.91          |
| (1,1729) | 1:B:150:LYS:HG2  | 1:B:151:GLN:H    | 6        | 0.91          |
| (1,1729) | 1:B:150:LYS:HG3  | 1:B:151:GLN:H    | 6        | 0.91          |
| (1,1708) | 1:B:147:GLY:HA2  | 1:B:132:THR:HA   | 4        | 0.91          |
| (1,1518) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HA   | 5        | 0.91          |
| (1,1467) | 1:B:122:TYR:HA   | 1:B:123:ARG:HB3  | 2        | 0.91          |
| (1,1430) | 1:B:118:PHE:HB2  | 1:B:118:PHE:H    | 3        | 0.91          |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB2  | 9        | 0.91          |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB3  | 9        | 0.91          |
| (1,1380) | 1:B:114:ILE:HA   | 1:B:114:ILE:HB   | 3        | 0.91          |
| (1,1371) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HD2  | 8        | 0.91          |
| (1,1371) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HD2  | 8        | 0.91          |
| (1,1371) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HD2  | 8        | 0.91          |
| (1,126)  | 1:A:78:ASN:H     | 1:A:78:ASN:HD22  | 4        | 0.91          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG21  | 3        | 0.91          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG22  | 3        | 0.91          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG23  | 3        | 0.91          |
| (1,862)  | 1:A:150:LYS:HG2  | 1:A:151:GLN:H    | 6        | 0.9           |
| (1,862)  | 1:A:150:LYS:HG3  | 1:A:151:GLN:H    | 6        | 0.9           |
| (1,651)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HA   | 9        | 0.9           |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG21 | 9        | 0.9           |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG22 | 9        | 0.9           |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG23 | 9        | 0.9           |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG11  | 6        | 0.9           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,604)  | 1:A:123:ARG:HB2 | 1:A:97:VAL:HG12 | 6        | 0.9           |
| (1,604)  | 1:A:123:ARG:HB2 | 1:A:97:VAL:HG13 | 6        | 0.9           |
| (1,604)  | 1:A:123:ARG:HB2 | 1:A:97:VAL:HG21 | 6        | 0.9           |
| (1,604)  | 1:A:123:ARG:HB2 | 1:A:97:VAL:HG22 | 6        | 0.9           |
| (1,604)  | 1:A:123:ARG:HB2 | 1:A:97:VAL:HG23 | 6        | 0.9           |
| (1,600)  | 1:A:122:TYR:HA  | 1:A:123:ARG:HB3 | 2        | 0.9           |
| (1,584)  | 1:A:121:LYS:HA  | 1:A:120:ARG:HB2 | 2        | 0.9           |
| (1,584)  | 1:A:121:LYS:HA  | 1:A:120:ARG:HB3 | 2        | 0.9           |
| (1,550)  | 1:A:118:PHE:HE1 | 1:A:102:GLY:H   | 5        | 0.9           |
| (1,550)  | 1:A:118:PHE:HE2 | 1:A:102:GLY:H   | 5        | 0.9           |
| (1,490)  | 1:A:113:PHE:HD1 | 1:A:113:PHE:HB2 | 2        | 0.9           |
| (1,490)  | 1:A:113:PHE:HD2 | 1:A:113:PHE:HB2 | 2        | 0.9           |
| (1,433)  | 1:A:107:ARG:HB3 | 1:A:108:GLN:H   | 1        | 0.9           |
| (1,385)  | 1:A:102:GLY:HA2 | 1:A:84:PHE:HZ   | 6        | 0.9           |
| (1,246)  | 1:A:89:LEU:H    | 1:A:89:LEU:HG   | 8        | 0.9           |
| (1,188)  | 1:A:83:HIS:H    | 1:A:141:GLY:HA2 | 4        | 0.9           |
| (1,1518) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HA  | 9        | 0.9           |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG11 | 6        | 0.9           |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG12 | 6        | 0.9           |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG13 | 6        | 0.9           |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG21 | 6        | 0.9           |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG22 | 6        | 0.9           |
| (1,1471) | 1:B:123:ARG:HB2 | 1:B:97:VAL:HG23 | 6        | 0.9           |
| (1,1451) | 1:B:121:LYS:HA  | 1:B:120:ARG:HB2 | 2        | 0.9           |
| (1,1451) | 1:B:121:LYS:HA  | 1:B:120:ARG:HB3 | 2        | 0.9           |
| (1,1417) | 1:B:118:PHE:HE1 | 1:B:102:GLY:H   | 5        | 0.9           |
| (1,1417) | 1:B:118:PHE:HE2 | 1:B:102:GLY:H   | 5        | 0.9           |
| (1,1357) | 1:B:113:PHE:HD1 | 1:B:113:PHE:HB2 | 2        | 0.9           |
| (1,1357) | 1:B:113:PHE:HD2 | 1:B:113:PHE:HB2 | 2        | 0.9           |
| (1,1300) | 1:B:107:ARG:HB3 | 1:B:108:GLN:H   | 1        | 0.9           |
| (1,1113) | 1:B:89:LEU:H    | 1:B:89:LEU:HG   | 8        | 0.9           |
| (1,1055) | 1:B:83:HIS:H    | 1:B:141:GLY:HA2 | 4        | 0.9           |
| (1,859)  | 1:A:150:LYS:H   | 1:A:150:LYS:HG2 | 8        | 0.89          |
| (1,859)  | 1:A:150:LYS:H   | 1:A:150:LYS:HG3 | 8        | 0.89          |
| (1,846)  | 1:A:147:GLY:HA2 | 1:A:147:GLY:HA3 | 1        | 0.89          |
| (1,651)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HA  | 6        | 0.89          |
| (1,598)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:H   | 7        | 0.89          |
| (1,598)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:H   | 7        | 0.89          |
| (1,597)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:H   | 7        | 0.89          |
| (1,597)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:H   | 7        | 0.89          |
| (1,550)  | 1:A:118:PHE:HE1 | 1:A:102:GLY:H   | 8        | 0.89          |
| (1,550)  | 1:A:118:PHE:HE2 | 1:A:102:GLY:H   | 8        | 0.89          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,513)  | 1:A:114:ILE:HA  | 1:A:114:ILE:HB   | 1        | 0.89          |
| (1,506)  | 1:A:114:ILE:HB  | 1:A:107:ARG:HD3  | 9        | 0.89          |
| (1,381)  | 1:A:101:HIS:HA  | 1:A:102:GLY:H    | 4        | 0.89          |
| (1,246)  | 1:A:89:LEU:H    | 1:A:89:LEU:HG    | 2        | 0.89          |
| (1,223)  | 1:A:87:GLU:H    | 1:A:88:GLU:HB2   | 6        | 0.89          |
| (1,223)  | 1:A:87:GLU:H    | 1:A:88:GLU:HB3   | 6        | 0.89          |
| (1,1761) | 1:A:120:ARG:HB2 | 1:B:111:HIS:H    | 2        | 0.89          |
| (1,1761) | 1:A:120:ARG:HB3 | 1:B:111:HIS:H    | 2        | 0.89          |
| (1,1729) | 1:B:150:LYS:HG2 | 1:B:151:GLN:H    | 1        | 0.89          |
| (1,1729) | 1:B:150:LYS:HG3 | 1:B:151:GLN:H    | 1        | 0.89          |
| (1,1726) | 1:B:150:LYS:H   | 1:B:150:LYS:HG2  | 8        | 0.89          |
| (1,1726) | 1:B:150:LYS:H   | 1:B:150:LYS:HG3  | 8        | 0.89          |
| (1,1713) | 1:B:147:GLY:HA2 | 1:B:147:GLY:HA3  | 1        | 0.89          |
| (1,1518) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HA   | 6        | 0.89          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG21 | 9        | 0.89          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG22 | 9        | 0.89          |
| (1,1516) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HG23 | 9        | 0.89          |
| (1,1465) | 1:B:122:TYR:HB2 | 1:B:122:TYR:H    | 7        | 0.89          |
| (1,1465) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H    | 7        | 0.89          |
| (1,1464) | 1:B:122:TYR:HB2 | 1:B:122:TYR:H    | 7        | 0.89          |
| (1,1464) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H    | 7        | 0.89          |
| (1,1417) | 1:B:118:PHE:HE1 | 1:B:102:GLY:H    | 8        | 0.89          |
| (1,1417) | 1:B:118:PHE:HE2 | 1:B:102:GLY:H    | 8        | 0.89          |
| (1,1380) | 1:B:114:ILE:HA  | 1:B:114:ILE:HB   | 1        | 0.89          |
| (1,1270) | 1:B:104:HIS:HA  | 1:B:104:HIS:HD2  | 1        | 0.89          |
| (1,1270) | 1:B:104:HIS:HA  | 1:B:104:HIS:HD2  | 9        | 0.89          |
| (1,1252) | 1:B:102:GLY:HA2 | 1:B:84:PHE:HZ    | 6        | 0.89          |
| (1,1248) | 1:B:101:HIS:HA  | 1:B:102:GLY:H    | 4        | 0.89          |
| (1,1113) | 1:B:89:LEU:H    | 1:B:89:LEU:HG    | 2        | 0.89          |
| (1,1090) | 1:B:87:GLU:H    | 1:B:88:GLU:HB2   | 6        | 0.89          |
| (1,1090) | 1:B:87:GLU:H    | 1:B:88:GLU:HB3   | 6        | 0.89          |
| (1,862)  | 1:A:150:LYS:HG2 | 1:A:151:GLN:H    | 1        | 0.88          |
| (1,862)  | 1:A:150:LYS:HG3 | 1:A:151:GLN:H    | 1        | 0.88          |
| (1,861)  | 1:A:150:LYS:HA  | 1:A:151:GLN:H    | 6        | 0.88          |
| (1,86)   | 1:A:77:VAL:HG21 | 1:A:75:PHE:HZ    | 1        | 0.88          |
| (1,86)   | 1:A:77:VAL:HG22 | 1:A:75:PHE:HZ    | 1        | 0.88          |
| (1,86)   | 1:A:77:VAL:HG23 | 1:A:75:PHE:HZ    | 1        | 0.88          |
| (1,846)  | 1:A:147:GLY:HA2 | 1:A:147:GLY:HA3  | 4        | 0.88          |
| (1,846)  | 1:A:147:GLY:HA2 | 1:A:147:GLY:HA3  | 7        | 0.88          |
| (1,846)  | 1:A:147:GLY:HA2 | 1:A:147:GLY:HA3  | 9        | 0.88          |
| (1,758)  | 1:A:138:SER:HA  | 1:A:141:GLY:H    | 6        | 0.88          |
| (1,734)  | 1:A:135:SER:H   | 1:A:134:THR:HB   | 6        | 0.88          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE1  | 1        | 0.88          |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE2  | 1        | 0.88          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE1  | 1        | 0.88          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE2  | 1        | 0.88          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE1  | 1        | 0.88          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE2  | 1        | 0.88          |
| (1,651)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HA  | 4        | 0.88          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD11 | 4        | 0.88          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD12 | 4        | 0.88          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD13 | 4        | 0.88          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD11 | 4        | 0.88          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD12 | 4        | 0.88          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD13 | 4        | 0.88          |
| (1,506)  | 1:A:114:ILE:HB   | 1:A:107:ARG:HD3 | 2        | 0.88          |
| (1,480)  | 1:A:112:GLY:HA3  | 1:A:113:PHE:H   | 8        | 0.88          |
| (1,445)  | 1:A:108:GLN:HA   | 1:A:113:PHE:H   | 9        | 0.88          |
| (1,433)  | 1:A:107:ARG:HB3  | 1:A:108:GLN:H   | 6        | 0.88          |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG2  | 1        | 0.88          |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG3  | 1        | 0.88          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD2  | 2        | 0.88          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD3  | 2        | 0.88          |
| (1,1748) | 1:A:115:SER:HB2  | 1:B:119:HIS:HB2 | 9        | 0.88          |
| (1,1748) | 1:A:115:SER:HB2  | 1:B:119:HIS:HB3 | 9        | 0.88          |
| (1,1745) | 1:A:114:ILE:H    | 1:B:121:LYS:H   | 1        | 0.88          |
| (1,1728) | 1:B:150:LYS:HA   | 1:B:151:GLN:H   | 6        | 0.88          |
| (1,1713) | 1:B:147:GLY:HA2  | 1:B:147:GLY:HA3 | 4        | 0.88          |
| (1,1713) | 1:B:147:GLY:HA2  | 1:B:147:GLY:HA3 | 7        | 0.88          |
| (1,1713) | 1:B:147:GLY:HA2  | 1:B:147:GLY:HA3 | 9        | 0.88          |
| (1,163)  | 1:A:81:VAL:HG21  | 1:A:83:HIS:H    | 4        | 0.88          |
| (1,163)  | 1:A:81:VAL:HG22  | 1:A:83:HIS:H    | 4        | 0.88          |
| (1,163)  | 1:A:81:VAL:HG23  | 1:A:83:HIS:H    | 4        | 0.88          |
| (1,1625) | 1:B:138:SER:HA   | 1:B:141:GLY:H   | 6        | 0.88          |
| (1,1601) | 1:B:135:SER:H    | 1:B:134:THR:HB  | 6        | 0.88          |
| (1,1373) | 1:B:114:ILE:HB   | 1:B:107:ARG:HD3 | 2        | 0.88          |
| (1,1373) | 1:B:114:ILE:HB   | 1:B:107:ARG:HD3 | 9        | 0.88          |
| (1,1347) | 1:B:112:GLY:HA3  | 1:B:113:PHE:H   | 8        | 0.88          |
| (1,1312) | 1:B:108:GLN:HA   | 1:B:113:PHE:H   | 9        | 0.88          |
| (1,1300) | 1:B:107:ARG:HB3  | 1:B:108:GLN:H   | 6        | 0.88          |
| (1,1260) | 1:B:103:LYS:H    | 1:B:88:GLU:HG2  | 1        | 0.88          |
| (1,1260) | 1:B:103:LYS:H    | 1:B:88:GLU:HG3  | 1        | 0.88          |
| (1,1030) | 1:B:81:VAL:HG21  | 1:B:83:HIS:H    | 4        | 0.88          |
| (1,1030) | 1:B:81:VAL:HG22  | 1:B:83:HIS:H    | 4        | 0.88          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1030) | 1:B:81:VAL:HG23  | 1:B:83:HIS:H    | 4        | 0.88          |
| (1,976)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:H    | 2        | 0.87          |
| (1,976)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:H    | 2        | 0.87          |
| (1,976)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:H    | 2        | 0.87          |
| (1,846)  | 1:A:147:GLY:HA2  | 1:A:147:GLY:HA3 | 5        | 0.87          |
| (1,843)  | 1:A:147:GLY:HA2  | 1:A:133:ILE:HB  | 1        | 0.87          |
| (1,758)  | 1:A:138:SER:HA   | 1:A:141:GLY:H   | 7        | 0.87          |
| (1,710)  | 1:A:132:THR:HB   | 1:A:148:PRO:HD2 | 3        | 0.87          |
| (1,710)  | 1:A:132:THR:HB   | 1:A:148:PRO:HD3 | 3        | 0.87          |
| (1,651)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HA  | 1        | 0.87          |
| (1,619)  | 1:A:124:ILE:HA   | 1:A:122:TYR:HD1 | 7        | 0.87          |
| (1,619)  | 1:A:124:ILE:HA   | 1:A:122:TYR:HD2 | 7        | 0.87          |
| (1,513)  | 1:A:114:ILE:HA   | 1:A:114:ILE:HB  | 8        | 0.87          |
| (1,490)  | 1:A:113:PHE:HD1  | 1:A:113:PHE:HB2 | 7        | 0.87          |
| (1,490)  | 1:A:113:PHE:HD2  | 1:A:113:PHE:HB2 | 7        | 0.87          |
| (1,403)  | 1:A:104:HIS:HA   | 1:A:104:HIS:HD2 | 2        | 0.87          |
| (1,397)  | 1:A:103:LYS:HG2  | 1:A:116:ARG:H   | 6        | 0.87          |
| (1,397)  | 1:A:103:LYS:HG3  | 1:A:116:ARG:H   | 6        | 0.87          |
| (1,1756) | 1:A:118:PHE:HA   | 1:B:117:GLU:H   | 7        | 0.87          |
| (1,1713) | 1:B:147:GLY:HA2  | 1:B:147:GLY:HA3 | 5        | 0.87          |
| (1,1710) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HB  | 1        | 0.87          |
| (1,1625) | 1:B:138:SER:HA   | 1:B:141:GLY:H   | 7        | 0.87          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE1  | 1        | 0.87          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE2  | 1        | 0.87          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE1  | 1        | 0.87          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE2  | 1        | 0.87          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE1  | 1        | 0.87          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE2  | 1        | 0.87          |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD2 | 3        | 0.87          |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD3 | 3        | 0.87          |
| (1,1518) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HA  | 1        | 0.87          |
| (1,1518) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HA  | 4        | 0.87          |
| (1,1486) | 1:B:124:ILE:HA   | 1:B:122:TYR:HD1 | 7        | 0.87          |
| (1,1486) | 1:B:124:ILE:HA   | 1:B:122:TYR:HD2 | 7        | 0.87          |
| (1,1380) | 1:B:114:ILE:HA   | 1:B:114:ILE:HB  | 8        | 0.87          |
| (1,1380) | 1:B:114:ILE:HA   | 1:B:114:ILE:HB  | 9        | 0.87          |
| (1,1357) | 1:B:113:PHE:HD1  | 1:B:113:PHE:HB2 | 7        | 0.87          |
| (1,1357) | 1:B:113:PHE:HD2  | 1:B:113:PHE:HB2 | 7        | 0.87          |
| (1,1264) | 1:B:103:LYS:HG2  | 1:B:116:ARG:H   | 6        | 0.87          |
| (1,1264) | 1:B:103:LYS:HG3  | 1:B:116:ARG:H   | 6        | 0.87          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD2  | 2        | 0.87          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD3  | 2        | 0.87          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,109)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:H     | 2        | 0.87          |
| (1,109)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:H     | 2        | 0.87          |
| (1,109)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:H     | 2        | 0.87          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG2   | 3        | 0.86          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG3   | 3        | 0.86          |
| (1,861)  | 1:A:150:LYS:HA   | 1:A:151:GLN:H    | 5        | 0.86          |
| (1,859)  | 1:A:150:LYS:H    | 1:A:150:LYS:HG2  | 2        | 0.86          |
| (1,859)  | 1:A:150:LYS:H    | 1:A:150:LYS:HG3  | 2        | 0.86          |
| (1,846)  | 1:A:147:GLY:HA2  | 1:A:147:GLY:HA3  | 8        | 0.86          |
| (1,813)  | 1:A:145:VAL:HA   | 1:A:135:SER:H    | 2        | 0.86          |
| (1,734)  | 1:A:135:SER:H    | 1:A:134:THR:HB   | 8        | 0.86          |
| (1,714)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HA   | 9        | 0.86          |
| (1,714)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HA   | 9        | 0.86          |
| (1,714)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HA   | 9        | 0.86          |
| (1,709)  | 1:A:132:THR:HB   | 1:A:147:GLY:HA3  | 4        | 0.86          |
| (1,703)  | 1:A:132:THR:HA   | 1:A:133:ILE:HA   | 8        | 0.86          |
| (1,568)  | 1:A:119:HIS:HB3  | 1:A:101:HIS:HA   | 4        | 0.86          |
| (1,559)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HD1  | 7        | 0.86          |
| (1,559)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HD2  | 7        | 0.86          |
| (1,527)  | 1:A:115:SER:HA   | 1:A:114:ILE:HD11 | 4        | 0.86          |
| (1,527)  | 1:A:115:SER:HA   | 1:A:114:ILE:HD12 | 4        | 0.86          |
| (1,527)  | 1:A:115:SER:HA   | 1:A:114:ILE:HD13 | 4        | 0.86          |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB2  | 2        | 0.86          |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB3  | 2        | 0.86          |
| (1,513)  | 1:A:114:ILE:HA   | 1:A:114:ILE:HB   | 5        | 0.86          |
| (1,513)  | 1:A:114:ILE:HA   | 1:A:114:ILE:HB   | 6        | 0.86          |
| (1,513)  | 1:A:114:ILE:HA   | 1:A:114:ILE:HB   | 9        | 0.86          |
| (1,480)  | 1:A:112:GLY:HA3  | 1:A:113:PHE:H    | 2        | 0.86          |
| (1,459)  | 1:A:111:HIS:H    | 1:A:110:GLU:H    | 2        | 0.86          |
| (1,458)  | 1:A:111:HIS:H    | 1:A:110:GLU:H    | 2        | 0.86          |
| (1,433)  | 1:A:107:ARG:HB3  | 1:A:108:GLN:H    | 4        | 0.86          |
| (1,367)  | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB2   | 8        | 0.86          |
| (1,367)  | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB3   | 8        | 0.86          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG2   | 3        | 0.86          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG3   | 3        | 0.86          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB2   | 7        | 0.86          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB3   | 7        | 0.86          |
| (1,1736) | 1:A:111:HIS:HB2  | 1:B:122:TYR:HE1  | 8        | 0.86          |
| (1,1736) | 1:A:111:HIS:HB2  | 1:B:122:TYR:HE2  | 8        | 0.86          |
| (1,1728) | 1:B:150:LYS:HA   | 1:B:151:GLN:H    | 5        | 0.86          |
| (1,1713) | 1:B:147:GLY:HA2  | 1:B:147:GLY:HA3  | 2        | 0.86          |
| (1,1713) | 1:B:147:GLY:HA2  | 1:B:147:GLY:HA3  | 8        | 0.86          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1680) | 1:B:145:VAL:HA   | 1:B:135:SER:H    | 2        | 0.86          |
| (1,1601) | 1:B:135:SER:H    | 1:B:134:THR:HB   | 8        | 0.86          |
| (1,1581) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HA   | 9        | 0.86          |
| (1,1581) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HA   | 9        | 0.86          |
| (1,1581) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HA   | 9        | 0.86          |
| (1,1576) | 1:B:132:THR:HB   | 1:B:147:GLY:HA3  | 4        | 0.86          |
| (1,1570) | 1:B:132:THR:HA   | 1:B:133:ILE:HA   | 8        | 0.86          |
| (1,1435) | 1:B:119:HIS:HB3  | 1:B:101:HIS:HA   | 4        | 0.86          |
| (1,1426) | 1:B:118:PHE:HA   | 1:B:118:PHE:HD1  | 7        | 0.86          |
| (1,1426) | 1:B:118:PHE:HA   | 1:B:118:PHE:HD2  | 7        | 0.86          |
| (1,1394) | 1:B:115:SER:HA   | 1:B:114:ILE:HD11 | 4        | 0.86          |
| (1,1394) | 1:B:115:SER:HA   | 1:B:114:ILE:HD12 | 4        | 0.86          |
| (1,1394) | 1:B:115:SER:HA   | 1:B:114:ILE:HD13 | 4        | 0.86          |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB2  | 2        | 0.86          |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB3  | 2        | 0.86          |
| (1,1380) | 1:B:114:ILE:HA   | 1:B:114:ILE:HB   | 5        | 0.86          |
| (1,1380) | 1:B:114:ILE:HA   | 1:B:114:ILE:HB   | 6        | 0.86          |
| (1,1347) | 1:B:112:GLY:HA3  | 1:B:113:PHE:H    | 2        | 0.86          |
| (1,1326) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 2        | 0.86          |
| (1,1325) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 2        | 0.86          |
| (1,1300) | 1:B:107:ARG:HB3  | 1:B:108:GLN:H    | 4        | 0.86          |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB2   | 8        | 0.86          |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB3   | 8        | 0.86          |
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB2   | 7        | 0.86          |
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB3   | 7        | 0.86          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG2   | 4        | 0.85          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG3   | 4        | 0.85          |
| (1,861)  | 1:A:150:LYS:HA   | 1:A:151:GLN:H    | 9        | 0.85          |
| (1,846)  | 1:A:147:GLY:HA2  | 1:A:147:GLY:HA3  | 2        | 0.85          |
| (1,846)  | 1:A:147:GLY:HA2  | 1:A:147:GLY:HA3  | 3        | 0.85          |
| (1,846)  | 1:A:147:GLY:HA2  | 1:A:147:GLY:HA3  | 6        | 0.85          |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE1   | 5        | 0.85          |
| (1,711)  | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE2   | 5        | 0.85          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE1   | 5        | 0.85          |
| (1,711)  | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE2   | 5        | 0.85          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE1   | 5        | 0.85          |
| (1,711)  | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE2   | 5        | 0.85          |
| (1,651)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HA   | 7        | 0.85          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD11 | 1        | 0.85          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD12 | 1        | 0.85          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD13 | 1        | 0.85          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD11 | 1        | 0.85          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD12 | 1        | 0.85          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD13 | 1        | 0.85          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD11 | 1        | 0.85          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD12 | 1        | 0.85          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD13 | 1        | 0.85          |
| (1,497)  | 1:A:113:PHE:HD1  | 1:A:113:PHE:H    | 3        | 0.85          |
| (1,497)  | 1:A:113:PHE:HD2  | 1:A:113:PHE:H    | 3        | 0.85          |
| (1,433)  | 1:A:107:ARG:HB3  | 1:A:108:GLN:H    | 2        | 0.85          |
| (1,433)  | 1:A:107:ARG:HB3  | 1:A:108:GLN:H    | 8        | 0.85          |
| (1,418)  | 1:A:105:GLU:HG2  | 1:A:115:SER:HB3  | 4        | 0.85          |
| (1,418)  | 1:A:105:GLU:HG3  | 1:A:115:SER:HB3  | 4        | 0.85          |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG2   | 6        | 0.85          |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG3   | 6        | 0.85          |
| (1,381)  | 1:A:101:HIS:HA   | 1:A:102:GLY:H    | 9        | 0.85          |
| (1,254)  | 1:A:89:LEU:HD11  | 1:A:91:VAL:HB    | 7        | 0.85          |
| (1,254)  | 1:A:89:LEU:HD12  | 1:A:91:VAL:HB    | 7        | 0.85          |
| (1,254)  | 1:A:89:LEU:HD13  | 1:A:91:VAL:HB    | 7        | 0.85          |
| (1,243)  | 1:A:89:LEU:HD11  | 1:A:88:GLU:H     | 1        | 0.85          |
| (1,243)  | 1:A:89:LEU:HD12  | 1:A:88:GLU:H     | 1        | 0.85          |
| (1,243)  | 1:A:89:LEU:HD13  | 1:A:88:GLU:H     | 1        | 0.85          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG2   | 4        | 0.85          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG3   | 4        | 0.85          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB2   | 8        | 0.85          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB3   | 8        | 0.85          |
| (1,1750) | 1:A:115:SER:HB2  | 1:B:119:HIS:HE1  | 2        | 0.85          |
| (1,1750) | 1:A:115:SER:HB2  | 1:B:119:HIS:HE1  | 3        | 0.85          |
| (1,1750) | 1:A:115:SER:HB2  | 1:B:119:HIS:HE1  | 8        | 0.85          |
| (1,1728) | 1:B:150:LYS:HA   | 1:B:151:GLN:H    | 9        | 0.85          |
| (1,1726) | 1:B:150:LYS:H    | 1:B:150:LYS:HG2  | 2        | 0.85          |
| (1,1726) | 1:B:150:LYS:H    | 1:B:150:LYS:HG3  | 2        | 0.85          |
| (1,1713) | 1:B:147:GLY:HA2  | 1:B:147:GLY:HA3  | 3        | 0.85          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE1   | 5        | 0.85          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE2   | 5        | 0.85          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE1   | 5        | 0.85          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE2   | 5        | 0.85          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE1   | 5        | 0.85          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE2   | 5        | 0.85          |
| (1,1518) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HA   | 7        | 0.85          |
| (1,1364) | 1:B:113:PHE:HD1  | 1:B:113:PHE:H    | 3        | 0.85          |
| (1,1364) | 1:B:113:PHE:HD2  | 1:B:113:PHE:H    | 3        | 0.85          |
| (1,1300) | 1:B:107:ARG:HB3  | 1:B:108:GLN:H    | 2        | 0.85          |
| (1,1300) | 1:B:107:ARG:HB3  | 1:B:108:GLN:H    | 8        | 0.85          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1285) | 1:B:105:GLU:HG2 | 1:B:115:SER:HB3  | 4        | 0.85          |
| (1,1285) | 1:B:105:GLU:HG3 | 1:B:115:SER:HB3  | 4        | 0.85          |
| (1,1260) | 1:B:103:LYS:H   | 1:B:88:GLU:HG2   | 6        | 0.85          |
| (1,1260) | 1:B:103:LYS:H   | 1:B:88:GLU:HG3   | 6        | 0.85          |
| (1,1248) | 1:B:101:HIS:HA  | 1:B:102:GLY:H    | 9        | 0.85          |
| (1,1121) | 1:B:89:LEU:HD11 | 1:B:91:VAL:HB    | 7        | 0.85          |
| (1,1121) | 1:B:89:LEU:HD12 | 1:B:91:VAL:HB    | 7        | 0.85          |
| (1,1121) | 1:B:89:LEU:HD13 | 1:B:91:VAL:HB    | 7        | 0.85          |
| (1,1110) | 1:B:89:LEU:HD11 | 1:B:88:GLU:H     | 1        | 0.85          |
| (1,1110) | 1:B:89:LEU:HD12 | 1:B:88:GLU:H     | 1        | 0.85          |
| (1,1110) | 1:B:89:LEU:HD13 | 1:B:88:GLU:H     | 1        | 0.85          |
| (1,1090) | 1:B:87:GLU:H    | 1:B:88:GLU:HB2   | 8        | 0.85          |
| (1,1090) | 1:B:87:GLU:H    | 1:B:88:GLU:HB3   | 8        | 0.85          |
| (1,710)  | 1:A:132:THR:HB  | 1:A:148:PRO:HD2  | 2        | 0.84          |
| (1,710)  | 1:A:132:THR:HB  | 1:A:148:PRO:HD3  | 2        | 0.84          |
| (1,513)  | 1:A:114:ILE:HA  | 1:A:114:ILE:HB   | 2        | 0.84          |
| (1,513)  | 1:A:114:ILE:HA  | 1:A:114:ILE:HB   | 7        | 0.84          |
| (1,480)  | 1:A:112:GLY:HA3 | 1:A:113:PHE:H    | 4        | 0.84          |
| (1,480)  | 1:A:112:GLY:HA3 | 1:A:113:PHE:H    | 9        | 0.84          |
| (1,452)  | 1:A:109:ASP:H   | 1:A:114:ILE:HG13 | 4        | 0.84          |
| (1,433)  | 1:A:107:ARG:HB3 | 1:A:108:GLN:H    | 3        | 0.84          |
| (1,433)  | 1:A:107:ARG:HB3 | 1:A:108:GLN:H    | 5        | 0.84          |
| (1,393)  | 1:A:103:LYS:H   | 1:A:88:GLU:HG2   | 9        | 0.84          |
| (1,393)  | 1:A:103:LYS:H   | 1:A:88:GLU:HG3   | 9        | 0.84          |
| (1,338)  | 1:A:98:ILE:HG21 | 1:A:98:ILE:HB    | 7        | 0.84          |
| (1,338)  | 1:A:98:ILE:HG22 | 1:A:98:ILE:HB    | 7        | 0.84          |
| (1,338)  | 1:A:98:ILE:HG23 | 1:A:98:ILE:HB    | 7        | 0.84          |
| (1,246)  | 1:A:89:LEU:H    | 1:A:89:LEU:HG    | 6        | 0.84          |
| (1,223)  | 1:A:87:GLU:H    | 1:A:88:GLU:HB2   | 3        | 0.84          |
| (1,223)  | 1:A:87:GLU:H    | 1:A:88:GLU:HB3   | 3        | 0.84          |
| (1,1713) | 1:B:147:GLY:HA2 | 1:B:147:GLY:HA3  | 6        | 0.84          |
| (1,1577) | 1:B:132:THR:HB  | 1:B:148:PRO:HD2  | 2        | 0.84          |
| (1,1577) | 1:B:132:THR:HB  | 1:B:148:PRO:HD3  | 2        | 0.84          |
| (1,1380) | 1:B:114:ILE:HA  | 1:B:114:ILE:HB   | 2        | 0.84          |
| (1,1380) | 1:B:114:ILE:HA  | 1:B:114:ILE:HB   | 7        | 0.84          |
| (1,1347) | 1:B:112:GLY:HA3 | 1:B:113:PHE:H    | 4        | 0.84          |
| (1,1347) | 1:B:112:GLY:HA3 | 1:B:113:PHE:H    | 9        | 0.84          |
| (1,1319) | 1:B:109:ASP:H   | 1:B:114:ILE:HG13 | 4        | 0.84          |
| (1,1300) | 1:B:107:ARG:HB3 | 1:B:108:GLN:H    | 3        | 0.84          |
| (1,1300) | 1:B:107:ARG:HB3 | 1:B:108:GLN:H    | 5        | 0.84          |
| (1,1300) | 1:B:107:ARG:HB3 | 1:B:108:GLN:H    | 9        | 0.84          |
| (1,1260) | 1:B:103:LYS:H   | 1:B:88:GLU:HG2   | 9        | 0.84          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1260) | 1:B:103:LYS:H    | 1:B:88:GLU:HG3   | 9        | 0.84          |
| (1,1250) | 1:B:101:HIS:HA   | 1:B:119:HIS:HD2  | 9        | 0.84          |
| (1,1113) | 1:B:89:LEU:H     | 1:B:89:LEU:HG    | 6        | 0.84          |
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB2   | 3        | 0.84          |
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB3   | 3        | 0.84          |
| (1,932)  | 1:B:76:SER:HB2   | 1:B:144:THR:HG21 | 5        | 0.83          |
| (1,932)  | 1:B:76:SER:HB2   | 1:B:144:THR:HG22 | 5        | 0.83          |
| (1,932)  | 1:B:76:SER:HB2   | 1:B:144:THR:HG23 | 5        | 0.83          |
| (1,710)  | 1:A:132:THR:HB   | 1:A:148:PRO:HD2  | 5        | 0.83          |
| (1,710)  | 1:A:132:THR:HB   | 1:A:148:PRO:HD3  | 5        | 0.83          |
| (1,65)   | 1:A:76:SER:HB2   | 1:A:144:THR:HG21 | 5        | 0.83          |
| (1,65)   | 1:A:76:SER:HB2   | 1:A:144:THR:HG22 | 5        | 0.83          |
| (1,65)   | 1:A:76:SER:HB2   | 1:A:144:THR:HG23 | 5        | 0.83          |
| (1,544)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 3        | 0.83          |
| (1,543)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 3        | 0.83          |
| (1,504)  | 1:A:114:ILE:HD11 | 1:A:107:ARG:HD2  | 3        | 0.83          |
| (1,504)  | 1:A:114:ILE:HD12 | 1:A:107:ARG:HD2  | 3        | 0.83          |
| (1,504)  | 1:A:114:ILE:HD13 | 1:A:107:ARG:HD2  | 3        | 0.83          |
| (1,433)  | 1:A:107:ARG:HB3  | 1:A:108:GLN:H    | 9        | 0.83          |
| (1,288)  | 1:A:93:VAL:HA    | 1:A:99:GLU:H     | 1        | 0.83          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG21  | 1        | 0.83          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG22  | 1        | 0.83          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG23  | 1        | 0.83          |
| (1,236)  | 1:A:89:LEU:HD21  | 1:A:85:SER:HB3   | 1        | 0.83          |
| (1,236)  | 1:A:89:LEU:HD22  | 1:A:85:SER:HB3   | 1        | 0.83          |
| (1,236)  | 1:A:89:LEU:HD23  | 1:A:85:SER:HB3   | 1        | 0.83          |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD2  | 5        | 0.83          |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD3  | 5        | 0.83          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD11 | 1        | 0.83          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD12 | 1        | 0.83          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD13 | 1        | 0.83          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD11 | 1        | 0.83          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD12 | 1        | 0.83          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD13 | 1        | 0.83          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD11 | 1        | 0.83          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD12 | 1        | 0.83          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD13 | 1        | 0.83          |
| (1,1411) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA   | 3        | 0.83          |
| (1,1410) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA   | 3        | 0.83          |
| (1,1155) | 1:B:93:VAL:HA    | 1:B:99:GLU:H     | 1        | 0.83          |
| (1,1103) | 1:B:89:LEU:HD21  | 1:B:85:SER:HB3   | 1        | 0.83          |
| (1,1103) | 1:B:89:LEU:HD22  | 1:B:85:SER:HB3   | 1        | 0.83          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1103) | 1:B:89:LEU:HD23  | 1:B:85:SER:HB3  | 1        | 0.83          |
| (1,982)  | 1:B:77:VAL:HG11  | 1:B:145:VAL:H   | 2        | 0.82          |
| (1,982)  | 1:B:77:VAL:HG12  | 1:B:145:VAL:H   | 2        | 0.82          |
| (1,982)  | 1:B:77:VAL:HG13  | 1:B:145:VAL:H   | 2        | 0.82          |
| (1,979)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HD1 | 5        | 0.82          |
| (1,979)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HD2 | 5        | 0.82          |
| (1,979)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HD1 | 5        | 0.82          |
| (1,979)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HD2 | 5        | 0.82          |
| (1,979)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HD1 | 5        | 0.82          |
| (1,979)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HD2 | 5        | 0.82          |
| (1,758)  | 1:A:138:SER:HA   | 1:A:141:GLY:H   | 4        | 0.82          |
| (1,651)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HA  | 3        | 0.82          |
| (1,632)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA  | 4        | 0.82          |
| (1,632)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA  | 4        | 0.82          |
| (1,632)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA  | 4        | 0.82          |
| (1,631)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA  | 4        | 0.82          |
| (1,631)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA  | 4        | 0.82          |
| (1,631)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA  | 4        | 0.82          |
| (1,595)  | 1:A:122:TYR:HD1  | 1:A:122:TYR:H   | 1        | 0.82          |
| (1,595)  | 1:A:122:TYR:HD2  | 1:A:122:TYR:H   | 1        | 0.82          |
| (1,558)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HZ  | 3        | 0.82          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB2 | 4        | 0.82          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB3 | 4        | 0.82          |
| (1,433)  | 1:A:107:ARG:HB3  | 1:A:108:GLN:H   | 7        | 0.82          |
| (1,403)  | 1:A:104:HIS:HA   | 1:A:104:HIS:HD2 | 3        | 0.82          |
| (1,403)  | 1:A:104:HIS:HA   | 1:A:104:HIS:HD2 | 9        | 0.82          |
| (1,355)  | 1:A:99:GLU:HB2   | 1:A:121:LYS:HG2 | 9        | 0.82          |
| (1,355)  | 1:A:99:GLU:HB2   | 1:A:121:LYS:HG3 | 9        | 0.82          |
| (1,355)  | 1:A:99:GLU:HB3   | 1:A:121:LYS:HG2 | 9        | 0.82          |
| (1,355)  | 1:A:99:GLU:HB3   | 1:A:121:LYS:HG3 | 9        | 0.82          |
| (1,338)  | 1:A:98:ILE:HG21  | 1:A:98:ILE:HB   | 5        | 0.82          |
| (1,338)  | 1:A:98:ILE:HG22  | 1:A:98:ILE:HB   | 5        | 0.82          |
| (1,338)  | 1:A:98:ILE:HG23  | 1:A:98:ILE:HB   | 5        | 0.82          |
| (1,338)  | 1:A:98:ILE:HG21  | 1:A:98:ILE:HB   | 9        | 0.82          |
| (1,338)  | 1:A:98:ILE:HG22  | 1:A:98:ILE:HB   | 9        | 0.82          |
| (1,338)  | 1:A:98:ILE:HG23  | 1:A:98:ILE:HB   | 9        | 0.82          |
| (1,256)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2 | 5        | 0.82          |
| (1,255)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2 | 5        | 0.82          |
| (1,199)  | 1:A:84:PHE:HB2   | 1:A:85:SER:H    | 9        | 0.82          |
| (1,199)  | 1:A:84:PHE:HB3   | 1:A:85:SER:H    | 9        | 0.82          |
| (1,1770) | 1:A:123:ARG:HD2  | 1:B:113:PHE:H   | 9        | 0.82          |
| (1,1770) | 1:A:123:ARG:HD3  | 1:B:113:PHE:H   | 9        | 0.82          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1733) | 1:B:152:VAL:H    | 1:B:151:GLN:H   | 7        | 0.82          |
| (1,167)  | 1:A:81:VAL:H     | 1:A:141:GLY:HA2 | 2        | 0.82          |
| (1,1625) | 1:B:138:SER:HA   | 1:B:141:GLY:H   | 4        | 0.82          |
| (1,1518) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HA  | 3        | 0.82          |
| (1,1462) | 1:B:122:TYR:HD1  | 1:B:122:TYR:H   | 1        | 0.82          |
| (1,1462) | 1:B:122:TYR:HD2  | 1:B:122:TYR:H   | 1        | 0.82          |
| (1,1425) | 1:B:118:PHE:HA   | 1:B:118:PHE:HZ  | 3        | 0.82          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB2 | 4        | 0.82          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB3 | 4        | 0.82          |
| (1,1371) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HD2 | 3        | 0.82          |
| (1,1371) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HD2 | 3        | 0.82          |
| (1,1371) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HD2 | 3        | 0.82          |
| (1,1222) | 1:B:99:GLU:HB2   | 1:B:121:LYS:HG2 | 9        | 0.82          |
| (1,1222) | 1:B:99:GLU:HB2   | 1:B:121:LYS:HG3 | 9        | 0.82          |
| (1,1222) | 1:B:99:GLU:HB3   | 1:B:121:LYS:HG2 | 9        | 0.82          |
| (1,1222) | 1:B:99:GLU:HB3   | 1:B:121:LYS:HG3 | 9        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG21  | 1:B:98:ILE:HB   | 2        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG22  | 1:B:98:ILE:HB   | 2        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG23  | 1:B:98:ILE:HB   | 2        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG21  | 1:B:98:ILE:HB   | 5        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG22  | 1:B:98:ILE:HB   | 5        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG23  | 1:B:98:ILE:HB   | 5        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG21  | 1:B:98:ILE:HB   | 7        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG22  | 1:B:98:ILE:HB   | 7        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG23  | 1:B:98:ILE:HB   | 7        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG21  | 1:B:98:ILE:HB   | 9        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG22  | 1:B:98:ILE:HB   | 9        | 0.82          |
| (1,1205) | 1:B:98:ILE:HG23  | 1:B:98:ILE:HB   | 9        | 0.82          |
| (1,115)  | 1:A:77:VAL:HG11  | 1:A:145:VAL:H   | 2        | 0.82          |
| (1,115)  | 1:A:77:VAL:HG12  | 1:A:145:VAL:H   | 2        | 0.82          |
| (1,115)  | 1:A:77:VAL:HG13  | 1:A:145:VAL:H   | 2        | 0.82          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG21 | 1        | 0.82          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG22 | 1        | 0.82          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG23 | 1        | 0.82          |
| (1,1123) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2 | 5        | 0.82          |
| (1,1122) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2 | 5        | 0.82          |
| (1,1066) | 1:B:84:PHE:HB2   | 1:B:85:SER:H    | 9        | 0.82          |
| (1,1066) | 1:B:84:PHE:HB3   | 1:B:85:SER:H    | 9        | 0.82          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD11 | 4        | 0.81          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD12 | 4        | 0.81          |
| (1,919)  | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD13 | 4        | 0.81          |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD11 | 4        | 0.81          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD12 | 4        | 0.81          |
| (1,919)  | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD13 | 4        | 0.81          |
| (1,866)  | 1:A:152:VAL:H    | 1:A:151:GLN:H   | 7        | 0.81          |
| (1,734)  | 1:A:135:SER:H    | 1:A:134:THR:HB  | 1        | 0.81          |
| (1,709)  | 1:A:132:THR:HB   | 1:A:147:GLY:HA3 | 7        | 0.81          |
| (1,600)  | 1:A:122:TYR:HA   | 1:A:123:ARG:HB3 | 1        | 0.81          |
| (1,564)  | 1:A:118:PHE:HD1  | 1:A:118:PHE:H   | 4        | 0.81          |
| (1,564)  | 1:A:118:PHE:HD2  | 1:A:118:PHE:H   | 4        | 0.81          |
| (1,564)  | 1:A:118:PHE:HD1  | 1:A:118:PHE:H   | 5        | 0.81          |
| (1,564)  | 1:A:118:PHE:HD2  | 1:A:118:PHE:H   | 5        | 0.81          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB2 | 5        | 0.81          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB3 | 5        | 0.81          |
| (1,383)  | 1:A:101:HIS:HA   | 1:A:119:HIS:HD2 | 9        | 0.81          |
| (1,346)  | 1:A:98:ILE:H     | 1:A:122:TYR:H   | 2        | 0.81          |
| (1,345)  | 1:A:98:ILE:H     | 1:A:122:TYR:H   | 2        | 0.81          |
| (1,338)  | 1:A:98:ILE:HG21  | 1:A:98:ILE:HB   | 2        | 0.81          |
| (1,338)  | 1:A:98:ILE:HG22  | 1:A:98:ILE:HB   | 2        | 0.81          |
| (1,338)  | 1:A:98:ILE:HG23  | 1:A:98:ILE:HB   | 2        | 0.81          |
| (1,338)  | 1:A:98:ILE:HG21  | 1:A:98:ILE:HB   | 4        | 0.81          |
| (1,338)  | 1:A:98:ILE:HG22  | 1:A:98:ILE:HB   | 4        | 0.81          |
| (1,338)  | 1:A:98:ILE:HG23  | 1:A:98:ILE:HB   | 4        | 0.81          |
| (1,338)  | 1:A:98:ILE:HG21  | 1:A:98:ILE:HB   | 6        | 0.81          |
| (1,338)  | 1:A:98:ILE:HG22  | 1:A:98:ILE:HB   | 6        | 0.81          |
| (1,338)  | 1:A:98:ILE:HG23  | 1:A:98:ILE:HB   | 6        | 0.81          |
| (1,269)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG11 | 6        | 0.81          |
| (1,269)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG12 | 6        | 0.81          |
| (1,269)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG13 | 6        | 0.81          |
| (1,256)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2 | 8        | 0.81          |
| (1,255)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2 | 8        | 0.81          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB2  | 4        | 0.81          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB3  | 4        | 0.81          |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG2  | 9        | 0.81          |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG3  | 9        | 0.81          |
| (1,181)  | 1:A:83:HIS:HB2   | 1:A:84:PHE:HB2  | 6        | 0.81          |
| (1,181)  | 1:A:83:HIS:HB2   | 1:A:84:PHE:HB3  | 6        | 0.81          |
| (1,1768) | 1:A:122:TYR:HA   | 1:B:112:GLY:H   | 6        | 0.81          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE1 | 2        | 0.81          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE2 | 2        | 0.81          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE1 | 2        | 0.81          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE2 | 2        | 0.81          |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE1 | 2        | 0.81          |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE2 | 2        | 0.81          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1601) | 1:B:135:SER:H    | 1:B:134:THR:HB  | 1        | 0.81          |
| (1,1576) | 1:B:132:THR:HB   | 1:B:147:GLY:HA3 | 7        | 0.81          |
| (1,1499) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA  | 4        | 0.81          |
| (1,1499) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA  | 4        | 0.81          |
| (1,1499) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA  | 4        | 0.81          |
| (1,1498) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA  | 4        | 0.81          |
| (1,1498) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA  | 4        | 0.81          |
| (1,1498) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA  | 4        | 0.81          |
| (1,1467) | 1:B:122:TYR:HA   | 1:B:123:ARG:HB3 | 1        | 0.81          |
| (1,1431) | 1:B:118:PHE:HD1  | 1:B:118:PHE:H   | 4        | 0.81          |
| (1,1431) | 1:B:118:PHE:HD2  | 1:B:118:PHE:H   | 4        | 0.81          |
| (1,1431) | 1:B:118:PHE:HD1  | 1:B:118:PHE:H   | 5        | 0.81          |
| (1,1431) | 1:B:118:PHE:HD2  | 1:B:118:PHE:H   | 5        | 0.81          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB2 | 5        | 0.81          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB3 | 5        | 0.81          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD1 | 8        | 0.81          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD2 | 8        | 0.81          |
| (1,1300) | 1:B:107:ARG:HB3  | 1:B:108:GLN:H   | 7        | 0.81          |
| (1,1270) | 1:B:104:HIS:HA   | 1:B:104:HIS:HD2 | 3        | 0.81          |
| (1,1213) | 1:B:98:ILE:H     | 1:B:122:TYR:H   | 2        | 0.81          |
| (1,1212) | 1:B:98:ILE:H     | 1:B:122:TYR:H   | 2        | 0.81          |
| (1,1205) | 1:B:98:ILE:HG21  | 1:B:98:ILE:HB   | 6        | 0.81          |
| (1,1205) | 1:B:98:ILE:HG22  | 1:B:98:ILE:HB   | 6        | 0.81          |
| (1,1205) | 1:B:98:ILE:HG23  | 1:B:98:ILE:HB   | 6        | 0.81          |
| (1,1136) | 1:B:91:VAL:H     | 1:B:91:VAL:HG11 | 6        | 0.81          |
| (1,1136) | 1:B:91:VAL:H     | 1:B:91:VAL:HG12 | 6        | 0.81          |
| (1,1136) | 1:B:91:VAL:H     | 1:B:91:VAL:HG13 | 6        | 0.81          |
| (1,1123) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2 | 8        | 0.81          |
| (1,1122) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2 | 8        | 0.81          |
| (1,112)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HD1 | 5        | 0.81          |
| (1,112)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HD2 | 5        | 0.81          |
| (1,112)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HD1 | 5        | 0.81          |
| (1,112)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HD2 | 5        | 0.81          |
| (1,112)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HD1 | 5        | 0.81          |
| (1,112)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HD2 | 5        | 0.81          |
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB2  | 4        | 0.81          |
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB3  | 4        | 0.81          |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG2  | 9        | 0.81          |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG3  | 9        | 0.81          |
| (1,1048) | 1:B:83:HIS:HB2   | 1:B:84:PHE:HB2  | 6        | 0.81          |
| (1,1048) | 1:B:83:HIS:HB2   | 1:B:84:PHE:HB3  | 6        | 0.81          |
| (1,1034) | 1:B:81:VAL:H     | 1:B:141:GLY:HA2 | 2        | 0.81          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,930)  | 1:B:76:SER:HB2  | 1:B:77:VAL:H    | 9        | 0.8           |
| (1,917)  | 1:B:75:PHE:HD1  | 1:B:75:PHE:H    | 8        | 0.8           |
| (1,917)  | 1:B:75:PHE:HD2  | 1:B:75:PHE:H    | 8        | 0.8           |
| (1,863)  | 1:A:150:LYS:H   | 1:A:151:GLN:H   | 7        | 0.8           |
| (1,850)  | 1:A:147:GLY:HA2 | 1:A:149:ARG:H   | 8        | 0.8           |
| (1,843)  | 1:A:147:GLY:HA2 | 1:A:133:ILE:HB  | 9        | 0.8           |
| (1,710)  | 1:A:132:THR:HB  | 1:A:148:PRO:HD2 | 4        | 0.8           |
| (1,710)  | 1:A:132:THR:HB  | 1:A:148:PRO:HD3 | 4        | 0.8           |
| (1,710)  | 1:A:132:THR:HB  | 1:A:148:PRO:HD2 | 6        | 0.8           |
| (1,710)  | 1:A:132:THR:HB  | 1:A:148:PRO:HD3 | 6        | 0.8           |
| (1,651)  | 1:A:125:PRO:HD2 | 1:A:124:ILE:HA  | 8        | 0.8           |
| (1,63)   | 1:A:76:SER:HB2  | 1:A:77:VAL:H    | 9        | 0.8           |
| (1,605)  | 1:A:123:ARG:HD2 | 1:A:98:ILE:H    | 4        | 0.8           |
| (1,605)  | 1:A:123:ARG:HD3 | 1:A:98:ILE:H    | 4        | 0.8           |
| (1,538)  | 1:A:116:ARG:H   | 1:A:116:ARG:HB2 | 2        | 0.8           |
| (1,538)  | 1:A:116:ARG:H   | 1:A:116:ARG:HB3 | 2        | 0.8           |
| (1,50)   | 1:A:75:PHE:HD1  | 1:A:75:PHE:H    | 8        | 0.8           |
| (1,50)   | 1:A:75:PHE:HD2  | 1:A:75:PHE:H    | 8        | 0.8           |
| (1,480)  | 1:A:112:GLY:HA3 | 1:A:113:PHE:H   | 6        | 0.8           |
| (1,459)  | 1:A:111:HIS:H   | 1:A:110:GLU:H   | 7        | 0.8           |
| (1,458)  | 1:A:111:HIS:H   | 1:A:110:GLU:H   | 7        | 0.8           |
| (1,437)  | 1:A:107:ARG:HB2 | 1:A:113:PHE:HD1 | 8        | 0.8           |
| (1,437)  | 1:A:107:ARG:HB2 | 1:A:113:PHE:HD2 | 8        | 0.8           |
| (1,338)  | 1:A:98:ILE:HG21 | 1:A:98:ILE:HB   | 3        | 0.8           |
| (1,338)  | 1:A:98:ILE:HG22 | 1:A:98:ILE:HB   | 3        | 0.8           |
| (1,338)  | 1:A:98:ILE:HG23 | 1:A:98:ILE:HB   | 3        | 0.8           |
| (1,338)  | 1:A:98:ILE:HG21 | 1:A:98:ILE:HB   | 8        | 0.8           |
| (1,338)  | 1:A:98:ILE:HG22 | 1:A:98:ILE:HB   | 8        | 0.8           |
| (1,338)  | 1:A:98:ILE:HG23 | 1:A:98:ILE:HB   | 8        | 0.8           |
| (1,199)  | 1:A:84:PHE:HB2  | 1:A:85:SER:H    | 3        | 0.8           |
| (1,199)  | 1:A:84:PHE:HB3  | 1:A:85:SER:H    | 3        | 0.8           |
| (1,185)  | 1:A:83:HIS:HB3  | 1:A:104:HIS:HB2 | 4        | 0.8           |
| (1,1739) | 1:A:111:HIS:HA  | 1:B:122:TYR:HE1 | 1        | 0.8           |
| (1,1739) | 1:A:111:HIS:HA  | 1:B:122:TYR:HE2 | 1        | 0.8           |
| (1,1717) | 1:B:147:GLY:HA2 | 1:B:149:ARG:H   | 8        | 0.8           |
| (1,1710) | 1:B:147:GLY:HA2 | 1:B:133:ILE:HB  | 9        | 0.8           |
| (1,1577) | 1:B:132:THR:HB  | 1:B:148:PRO:HD2 | 4        | 0.8           |
| (1,1577) | 1:B:132:THR:HB  | 1:B:148:PRO:HD3 | 4        | 0.8           |
| (1,1577) | 1:B:132:THR:HB  | 1:B:148:PRO:HD2 | 6        | 0.8           |
| (1,1577) | 1:B:132:THR:HB  | 1:B:148:PRO:HD3 | 6        | 0.8           |
| (1,1570) | 1:B:132:THR:HA  | 1:B:133:ILE:HA  | 1        | 0.8           |
| (1,1518) | 1:B:125:PRO:HD2 | 1:B:124:ILE:HA  | 8        | 0.8           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1472) | 1:B:123:ARG:HD2 | 1:B:98:ILE:H    | 4        | 0.8           |
| (1,1472) | 1:B:123:ARG:HD3 | 1:B:98:ILE:H    | 4        | 0.8           |
| (1,1465) | 1:B:122:TYR:HB2 | 1:B:122:TYR:H   | 5        | 0.8           |
| (1,1465) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H   | 5        | 0.8           |
| (1,1464) | 1:B:122:TYR:HB2 | 1:B:122:TYR:H   | 5        | 0.8           |
| (1,1464) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H   | 5        | 0.8           |
| (1,1405) | 1:B:116:ARG:H   | 1:B:116:ARG:HB2 | 2        | 0.8           |
| (1,1405) | 1:B:116:ARG:H   | 1:B:116:ARG:HB3 | 2        | 0.8           |
| (1,1347) | 1:B:112:GLY:HA3 | 1:B:113:PHE:H   | 6        | 0.8           |
| (1,1326) | 1:B:111:HIS:H   | 1:B:110:GLU:H   | 7        | 0.8           |
| (1,1325) | 1:B:111:HIS:H   | 1:B:110:GLU:H   | 7        | 0.8           |
| (1,1205) | 1:B:98:ILE:HG21 | 1:B:98:ILE:HB   | 3        | 0.8           |
| (1,1205) | 1:B:98:ILE:HG22 | 1:B:98:ILE:HB   | 3        | 0.8           |
| (1,1205) | 1:B:98:ILE:HG23 | 1:B:98:ILE:HB   | 3        | 0.8           |
| (1,1205) | 1:B:98:ILE:HG21 | 1:B:98:ILE:HB   | 4        | 0.8           |
| (1,1205) | 1:B:98:ILE:HG22 | 1:B:98:ILE:HB   | 4        | 0.8           |
| (1,1205) | 1:B:98:ILE:HG23 | 1:B:98:ILE:HB   | 4        | 0.8           |
| (1,1205) | 1:B:98:ILE:HG21 | 1:B:98:ILE:HB   | 8        | 0.8           |
| (1,1205) | 1:B:98:ILE:HG22 | 1:B:98:ILE:HB   | 8        | 0.8           |
| (1,1205) | 1:B:98:ILE:HG23 | 1:B:98:ILE:HB   | 8        | 0.8           |
| (1,1066) | 1:B:84:PHE:HB2  | 1:B:85:SER:H    | 3        | 0.8           |
| (1,1066) | 1:B:84:PHE:HB3  | 1:B:85:SER:H    | 3        | 0.8           |
| (1,1052) | 1:B:83:HIS:HB3  | 1:B:104:HIS:HB2 | 4        | 0.8           |
| (1,958)  | 1:B:77:VAL:HG11 | 1:B:77:VAL:HB   | 2        | 0.79          |
| (1,958)  | 1:B:77:VAL:HG12 | 1:B:77:VAL:HB   | 2        | 0.79          |
| (1,958)  | 1:B:77:VAL:HG13 | 1:B:77:VAL:HB   | 2        | 0.79          |
| (1,958)  | 1:B:77:VAL:HG11 | 1:B:77:VAL:HB   | 6        | 0.79          |
| (1,958)  | 1:B:77:VAL:HG12 | 1:B:77:VAL:HB   | 6        | 0.79          |
| (1,958)  | 1:B:77:VAL:HG13 | 1:B:77:VAL:HB   | 6        | 0.79          |
| (1,958)  | 1:B:77:VAL:HG11 | 1:B:77:VAL:HB   | 7        | 0.79          |
| (1,958)  | 1:B:77:VAL:HG12 | 1:B:77:VAL:HB   | 7        | 0.79          |
| (1,958)  | 1:B:77:VAL:HG13 | 1:B:77:VAL:HB   | 7        | 0.79          |
| (1,951)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE1  | 3        | 0.79          |
| (1,951)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE2  | 3        | 0.79          |
| (1,951)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE3  | 3        | 0.79          |
| (1,951)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE1  | 3        | 0.79          |
| (1,951)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE2  | 3        | 0.79          |
| (1,951)  | 1:B:77:VAL:HG22 | 1:B:68:MET:HE3  | 3        | 0.79          |
| (1,951)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE1  | 3        | 0.79          |
| (1,951)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE2  | 3        | 0.79          |
| (1,951)  | 1:B:77:VAL:HG23 | 1:B:68:MET:HE3  | 3        | 0.79          |
| (1,946)  | 1:B:77:VAL:HG21 | 1:B:68:MET:HE1  | 3        | 0.79          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,946) | 1:B:77:VAL:HG21  | 1:B:68:MET:HE2   | 3        | 0.79          |
| (1,946) | 1:B:77:VAL:HG21  | 1:B:68:MET:HE3   | 3        | 0.79          |
| (1,946) | 1:B:77:VAL:HG22  | 1:B:68:MET:HE1   | 3        | 0.79          |
| (1,946) | 1:B:77:VAL:HG22  | 1:B:68:MET:HE2   | 3        | 0.79          |
| (1,946) | 1:B:77:VAL:HG22  | 1:B:68:MET:HE3   | 3        | 0.79          |
| (1,946) | 1:B:77:VAL:HG23  | 1:B:68:MET:HE1   | 3        | 0.79          |
| (1,946) | 1:B:77:VAL:HG23  | 1:B:68:MET:HE2   | 3        | 0.79          |
| (1,946) | 1:B:77:VAL:HG23  | 1:B:68:MET:HE3   | 3        | 0.79          |
| (1,932) | 1:B:76:SER:HB2   | 1:B:144:THR:HG21 | 6        | 0.79          |
| (1,932) | 1:B:76:SER:HB2   | 1:B:144:THR:HG22 | 6        | 0.79          |
| (1,932) | 1:B:76:SER:HB2   | 1:B:144:THR:HG23 | 6        | 0.79          |
| (1,91)  | 1:A:77:VAL:HG11  | 1:A:77:VAL:HB    | 2        | 0.79          |
| (1,91)  | 1:A:77:VAL:HG12  | 1:A:77:VAL:HB    | 2        | 0.79          |
| (1,91)  | 1:A:77:VAL:HG13  | 1:A:77:VAL:HB    | 2        | 0.79          |
| (1,91)  | 1:A:77:VAL:HG11  | 1:A:77:VAL:HB    | 6        | 0.79          |
| (1,91)  | 1:A:77:VAL:HG12  | 1:A:77:VAL:HB    | 6        | 0.79          |
| (1,91)  | 1:A:77:VAL:HG13  | 1:A:77:VAL:HB    | 6        | 0.79          |
| (1,91)  | 1:A:77:VAL:HG11  | 1:A:77:VAL:HB    | 7        | 0.79          |
| (1,91)  | 1:A:77:VAL:HG12  | 1:A:77:VAL:HB    | 7        | 0.79          |
| (1,91)  | 1:A:77:VAL:HG13  | 1:A:77:VAL:HB    | 7        | 0.79          |
| (1,734) | 1:A:135:SER:H    | 1:A:134:THR:HB   | 5        | 0.79          |
| (1,714) | 1:A:133:ILE:HD11 | 1:A:130:PRO:HA   | 4        | 0.79          |
| (1,714) | 1:A:133:ILE:HD12 | 1:A:130:PRO:HA   | 4        | 0.79          |
| (1,714) | 1:A:133:ILE:HD13 | 1:A:130:PRO:HA   | 4        | 0.79          |
| (1,703) | 1:A:132:THR:HA   | 1:A:133:ILE:HA   | 1        | 0.79          |
| (1,703) | 1:A:132:THR:HA   | 1:A:133:ILE:HA   | 5        | 0.79          |
| (1,703) | 1:A:132:THR:HA   | 1:A:133:ILE:HA   | 7        | 0.79          |
| (1,703) | 1:A:132:THR:HA   | 1:A:133:ILE:HA   | 9        | 0.79          |
| (1,65)  | 1:A:76:SER:HB2   | 1:A:144:THR:HG21 | 6        | 0.79          |
| (1,65)  | 1:A:76:SER:HB2   | 1:A:144:THR:HG22 | 6        | 0.79          |
| (1,65)  | 1:A:76:SER:HB2   | 1:A:144:THR:HG23 | 6        | 0.79          |
| (1,598) | 1:A:122:TYR:HB2  | 1:A:122:TYR:H    | 5        | 0.79          |
| (1,598) | 1:A:122:TYR:HB3  | 1:A:122:TYR:H    | 5        | 0.79          |
| (1,597) | 1:A:122:TYR:HB2  | 1:A:122:TYR:H    | 5        | 0.79          |
| (1,597) | 1:A:122:TYR:HB3  | 1:A:122:TYR:H    | 5        | 0.79          |
| (1,538) | 1:A:116:ARG:H    | 1:A:116:ARG:HB2  | 8        | 0.79          |
| (1,538) | 1:A:116:ARG:H    | 1:A:116:ARG:HB3  | 8        | 0.79          |
| (1,498) | 1:A:113:PHE:HB2  | 1:A:113:PHE:H    | 1        | 0.79          |
| (1,480) | 1:A:112:GLY:HA3  | 1:A:113:PHE:H    | 1        | 0.79          |
| (1,385) | 1:A:102:GLY:HA2  | 1:A:84:PHE:HZ    | 5        | 0.79          |
| (1,365) | 1:A:100:VAL:HG11 | 1:A:102:GLY:H    | 1        | 0.79          |
| (1,365) | 1:A:100:VAL:HG12 | 1:A:102:GLY:H    | 1        | 0.79          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,365)  | 1:A:100:VAL:HG13 | 1:A:102:GLY:H    | 1        | 0.79          |
| (1,338)  | 1:A:98:ILE:HG21  | 1:A:98:ILE:HB    | 1        | 0.79          |
| (1,338)  | 1:A:98:ILE:HG22  | 1:A:98:ILE:HB    | 1        | 0.79          |
| (1,338)  | 1:A:98:ILE:HG23  | 1:A:98:ILE:HB    | 1        | 0.79          |
| (1,246)  | 1:A:89:LEU:H     | 1:A:89:LEU:HG    | 1        | 0.79          |
| (1,1730) | 1:B:150:LYS:H    | 1:B:151:GLN:H    | 7        | 0.79          |
| (1,1601) | 1:B:135:SER:H    | 1:B:134:THR:HB   | 5        | 0.79          |
| (1,1581) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HA   | 4        | 0.79          |
| (1,1581) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HA   | 4        | 0.79          |
| (1,1581) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HA   | 4        | 0.79          |
| (1,1570) | 1:B:132:THR:HA   | 1:B:133:ILE:HA   | 5        | 0.79          |
| (1,1570) | 1:B:132:THR:HA   | 1:B:133:ILE:HA   | 7        | 0.79          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD11 | 3        | 0.79          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD12 | 3        | 0.79          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD13 | 3        | 0.79          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD11 | 3        | 0.79          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD12 | 3        | 0.79          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD13 | 3        | 0.79          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD11 | 3        | 0.79          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD12 | 3        | 0.79          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD13 | 3        | 0.79          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB2  | 8        | 0.79          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB3  | 8        | 0.79          |
| (1,1365) | 1:B:113:PHE:HB2  | 1:B:113:PHE:H    | 1        | 0.79          |
| (1,1347) | 1:B:112:GLY:HA3  | 1:B:113:PHE:H    | 1        | 0.79          |
| (1,1252) | 1:B:102:GLY:HA2  | 1:B:84:PHE:HZ    | 5        | 0.79          |
| (1,1232) | 1:B:100:VAL:HG11 | 1:B:102:GLY:H    | 1        | 0.79          |
| (1,1232) | 1:B:100:VAL:HG12 | 1:B:102:GLY:H    | 1        | 0.79          |
| (1,1232) | 1:B:100:VAL:HG13 | 1:B:102:GLY:H    | 1        | 0.79          |
| (1,1205) | 1:B:98:ILE:HG21  | 1:B:98:ILE:HB    | 1        | 0.79          |
| (1,1205) | 1:B:98:ILE:HG22  | 1:B:98:ILE:HB    | 1        | 0.79          |
| (1,1205) | 1:B:98:ILE:HG23  | 1:B:98:ILE:HB    | 1        | 0.79          |
| (1,1113) | 1:B:89:LEU:H     | 1:B:89:LEU:HG    | 1        | 0.79          |
| (1,1027) | 1:B:81:VAL:H     | 1:B:82:LYS:H     | 8        | 0.79          |
| (1,1026) | 1:B:81:VAL:H     | 1:B:82:LYS:H     | 8        | 0.79          |
| (1,1024) | 1:B:81:VAL:HG21  | 1:B:81:VAL:H     | 9        | 0.79          |
| (1,1024) | 1:B:81:VAL:HG22  | 1:B:81:VAL:H     | 9        | 0.79          |
| (1,1024) | 1:B:81:VAL:HG23  | 1:B:81:VAL:H     | 9        | 0.79          |
| (1,958)  | 1:B:77:VAL:HG11  | 1:B:77:VAL:HB    | 1        | 0.78          |
| (1,958)  | 1:B:77:VAL:HG12  | 1:B:77:VAL:HB    | 1        | 0.78          |
| (1,958)  | 1:B:77:VAL:HG13  | 1:B:77:VAL:HB    | 1        | 0.78          |
| (1,958)  | 1:B:77:VAL:HG11  | 1:B:77:VAL:HB    | 9        | 0.78          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,958) | 1:B:77:VAL:HG12  | 1:B:77:VAL:HB    | 9        | 0.78          |
| (1,958) | 1:B:77:VAL:HG13  | 1:B:77:VAL:HB    | 9        | 0.78          |
| (1,949) | 1:B:77:VAL:HG21  | 1:B:68:MET:HA    | 6        | 0.78          |
| (1,949) | 1:B:77:VAL:HG22  | 1:B:68:MET:HA    | 6        | 0.78          |
| (1,949) | 1:B:77:VAL:HG23  | 1:B:68:MET:HA    | 6        | 0.78          |
| (1,91)  | 1:A:77:VAL:HG11  | 1:A:77:VAL:HB    | 1        | 0.78          |
| (1,91)  | 1:A:77:VAL:HG12  | 1:A:77:VAL:HB    | 1        | 0.78          |
| (1,91)  | 1:A:77:VAL:HG13  | 1:A:77:VAL:HB    | 1        | 0.78          |
| (1,91)  | 1:A:77:VAL:HG11  | 1:A:77:VAL:HB    | 9        | 0.78          |
| (1,91)  | 1:A:77:VAL:HG12  | 1:A:77:VAL:HB    | 9        | 0.78          |
| (1,91)  | 1:A:77:VAL:HG13  | 1:A:77:VAL:HB    | 9        | 0.78          |
| (1,884) | 1:B:70:LEU:H     | 1:B:70:LEU:HB3   | 8        | 0.78          |
| (1,82)  | 1:A:77:VAL:HG21  | 1:A:68:MET:HA    | 6        | 0.78          |
| (1,82)  | 1:A:77:VAL:HG22  | 1:A:68:MET:HA    | 6        | 0.78          |
| (1,82)  | 1:A:77:VAL:HG23  | 1:A:68:MET:HA    | 6        | 0.78          |
| (1,710) | 1:A:132:THR:HB   | 1:A:148:PRO:HD2  | 9        | 0.78          |
| (1,710) | 1:A:132:THR:HB   | 1:A:148:PRO:HD3  | 9        | 0.78          |
| (1,703) | 1:A:132:THR:HA   | 1:A:133:ILE:HA   | 6        | 0.78          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD11 | 4        | 0.78          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD12 | 4        | 0.78          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD13 | 4        | 0.78          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD11 | 4        | 0.78          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD12 | 4        | 0.78          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD13 | 4        | 0.78          |
| (1,497) | 1:A:113:PHE:HD1  | 1:A:113:PHE:H    | 2        | 0.78          |
| (1,497) | 1:A:113:PHE:HD2  | 1:A:113:PHE:H    | 2        | 0.78          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG21 | 5        | 0.78          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG22 | 5        | 0.78          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG23 | 5        | 0.78          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG21 | 5        | 0.78          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG22 | 5        | 0.78          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG23 | 5        | 0.78          |
| (1,269) | 1:A:91:VAL:H     | 1:A:91:VAL:HG11  | 4        | 0.78          |
| (1,269) | 1:A:91:VAL:H     | 1:A:91:VAL:HG12  | 4        | 0.78          |
| (1,269) | 1:A:91:VAL:H     | 1:A:91:VAL:HG13  | 4        | 0.78          |
| (1,256) | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2  | 4        | 0.78          |
| (1,255) | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2  | 4        | 0.78          |
| (1,17)  | 1:A:70:LEU:H     | 1:A:70:LEU:HB3   | 8        | 0.78          |
| (1,166) | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD1  | 1        | 0.78          |
| (1,166) | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD2  | 1        | 0.78          |
| (1,166) | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD1  | 1        | 0.78          |
| (1,166) | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD2  | 1        | 0.78          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD1  | 1        | 0.78          |
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD2  | 1        | 0.78          |
| (1,160)  | 1:A:81:VAL:H     | 1:A:82:LYS:H     | 8        | 0.78          |
| (1,159)  | 1:A:81:VAL:H     | 1:A:82:LYS:H     | 8        | 0.78          |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD2  | 9        | 0.78          |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD3  | 9        | 0.78          |
| (1,1570) | 1:B:132:THR:HA   | 1:B:133:ILE:HA   | 6        | 0.78          |
| (1,1570) | 1:B:132:THR:HA   | 1:B:133:ILE:HA   | 9        | 0.78          |
| (1,157)  | 1:A:81:VAL:HG21  | 1:A:81:VAL:H     | 9        | 0.78          |
| (1,157)  | 1:A:81:VAL:HG22  | 1:A:81:VAL:H     | 9        | 0.78          |
| (1,157)  | 1:A:81:VAL:HG23  | 1:A:81:VAL:H     | 9        | 0.78          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD11 | 7        | 0.78          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD12 | 7        | 0.78          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD13 | 7        | 0.78          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD11 | 7        | 0.78          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD12 | 7        | 0.78          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD13 | 7        | 0.78          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD11 | 7        | 0.78          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD12 | 7        | 0.78          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD13 | 7        | 0.78          |
| (1,143)  | 1:A:79:LEU:HG    | 1:A:80:ASP:H     | 8        | 0.78          |
| (1,1364) | 1:B:113:PHE:HD1  | 1:B:113:PHE:H    | 2        | 0.78          |
| (1,1364) | 1:B:113:PHE:HD2  | 1:B:113:PHE:H    | 2        | 0.78          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG21 | 5        | 0.78          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG22 | 5        | 0.78          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG23 | 5        | 0.78          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG21 | 5        | 0.78          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG22 | 5        | 0.78          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG23 | 5        | 0.78          |
| (1,1136) | 1:B:91:VAL:H     | 1:B:91:VAL:HG11  | 4        | 0.78          |
| (1,1136) | 1:B:91:VAL:H     | 1:B:91:VAL:HG12  | 4        | 0.78          |
| (1,1136) | 1:B:91:VAL:H     | 1:B:91:VAL:HG13  | 4        | 0.78          |
| (1,1123) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2  | 4        | 0.78          |
| (1,1122) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2  | 4        | 0.78          |
| (1,1033) | 1:B:81:VAL:HG11  | 1:B:118:PHE:HD1  | 1        | 0.78          |
| (1,1033) | 1:B:81:VAL:HG11  | 1:B:118:PHE:HD2  | 1        | 0.78          |
| (1,1033) | 1:B:81:VAL:HG12  | 1:B:118:PHE:HD1  | 1        | 0.78          |
| (1,1033) | 1:B:81:VAL:HG12  | 1:B:118:PHE:HD2  | 1        | 0.78          |
| (1,1033) | 1:B:81:VAL:HG13  | 1:B:118:PHE:HD1  | 1        | 0.78          |
| (1,1033) | 1:B:81:VAL:HG13  | 1:B:118:PHE:HD2  | 1        | 0.78          |
| (1,1010) | 1:B:79:LEU:HG    | 1:B:80:ASP:H     | 8        | 0.78          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 6        | 0.77          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,962) | 1:B:77:VAL:HA   | 1:B:77:VAL:HG22 | 6        | 0.77          |
| (1,962) | 1:B:77:VAL:HA   | 1:B:77:VAL:HG23 | 6        | 0.77          |
| (1,958) | 1:B:77:VAL:HG11 | 1:B:77:VAL:HB   | 3        | 0.77          |
| (1,958) | 1:B:77:VAL:HG12 | 1:B:77:VAL:HB   | 3        | 0.77          |
| (1,958) | 1:B:77:VAL:HG13 | 1:B:77:VAL:HB   | 3        | 0.77          |
| (1,958) | 1:B:77:VAL:HG11 | 1:B:77:VAL:HB   | 4        | 0.77          |
| (1,958) | 1:B:77:VAL:HG12 | 1:B:77:VAL:HB   | 4        | 0.77          |
| (1,958) | 1:B:77:VAL:HG13 | 1:B:77:VAL:HB   | 4        | 0.77          |
| (1,958) | 1:B:77:VAL:HG11 | 1:B:77:VAL:HB   | 5        | 0.77          |
| (1,958) | 1:B:77:VAL:HG12 | 1:B:77:VAL:HB   | 5        | 0.77          |
| (1,958) | 1:B:77:VAL:HG13 | 1:B:77:VAL:HB   | 5        | 0.77          |
| (1,958) | 1:B:77:VAL:HG11 | 1:B:77:VAL:HB   | 8        | 0.77          |
| (1,958) | 1:B:77:VAL:HG12 | 1:B:77:VAL:HB   | 8        | 0.77          |
| (1,958) | 1:B:77:VAL:HG13 | 1:B:77:VAL:HB   | 8        | 0.77          |
| (1,956) | 1:B:77:VAL:HA   | 1:B:77:VAL:HG21 | 6        | 0.77          |
| (1,956) | 1:B:77:VAL:HA   | 1:B:77:VAL:HG22 | 6        | 0.77          |
| (1,956) | 1:B:77:VAL:HA   | 1:B:77:VAL:HG23 | 6        | 0.77          |
| (1,91)  | 1:A:77:VAL:HG11 | 1:A:77:VAL:HB   | 3        | 0.77          |
| (1,91)  | 1:A:77:VAL:HG12 | 1:A:77:VAL:HB   | 3        | 0.77          |
| (1,91)  | 1:A:77:VAL:HG13 | 1:A:77:VAL:HB   | 3        | 0.77          |
| (1,91)  | 1:A:77:VAL:HG11 | 1:A:77:VAL:HB   | 4        | 0.77          |
| (1,91)  | 1:A:77:VAL:HG12 | 1:A:77:VAL:HB   | 4        | 0.77          |
| (1,91)  | 1:A:77:VAL:HG13 | 1:A:77:VAL:HB   | 4        | 0.77          |
| (1,91)  | 1:A:77:VAL:HG11 | 1:A:77:VAL:HB   | 5        | 0.77          |
| (1,91)  | 1:A:77:VAL:HG12 | 1:A:77:VAL:HB   | 5        | 0.77          |
| (1,91)  | 1:A:77:VAL:HG13 | 1:A:77:VAL:HB   | 5        | 0.77          |
| (1,84)  | 1:A:77:VAL:HG21 | 1:A:68:MET:HE1  | 3        | 0.77          |
| (1,84)  | 1:A:77:VAL:HG21 | 1:A:68:MET:HE2  | 3        | 0.77          |
| (1,84)  | 1:A:77:VAL:HG21 | 1:A:68:MET:HE3  | 3        | 0.77          |
| (1,84)  | 1:A:77:VAL:HG22 | 1:A:68:MET:HE1  | 3        | 0.77          |
| (1,84)  | 1:A:77:VAL:HG22 | 1:A:68:MET:HE2  | 3        | 0.77          |
| (1,84)  | 1:A:77:VAL:HG22 | 1:A:68:MET:HE3  | 3        | 0.77          |
| (1,84)  | 1:A:77:VAL:HG23 | 1:A:68:MET:HE1  | 3        | 0.77          |
| (1,84)  | 1:A:77:VAL:HG23 | 1:A:68:MET:HE2  | 3        | 0.77          |
| (1,84)  | 1:A:77:VAL:HG23 | 1:A:68:MET:HE3  | 3        | 0.77          |
| (1,79)  | 1:A:77:VAL:HG21 | 1:A:68:MET:HE1  | 3        | 0.77          |
| (1,79)  | 1:A:77:VAL:HG21 | 1:A:68:MET:HE2  | 3        | 0.77          |
| (1,79)  | 1:A:77:VAL:HG21 | 1:A:68:MET:HE3  | 3        | 0.77          |
| (1,79)  | 1:A:77:VAL:HG22 | 1:A:68:MET:HE1  | 3        | 0.77          |
| (1,79)  | 1:A:77:VAL:HG22 | 1:A:68:MET:HE2  | 3        | 0.77          |
| (1,79)  | 1:A:77:VAL:HG22 | 1:A:68:MET:HE3  | 3        | 0.77          |
| (1,79)  | 1:A:77:VAL:HG23 | 1:A:68:MET:HE1  | 3        | 0.77          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,79)  | 1:A:77:VAL:HG23  | 1:A:68:MET:HE2   | 3        | 0.77          |
| (1,79)  | 1:A:77:VAL:HG23  | 1:A:68:MET:HE3   | 3        | 0.77          |
| (1,744) | 1:A:135:SER:HB3  | 1:A:146:ASP:H    | 1        | 0.77          |
| (1,723) | 1:A:133:ILE:HG21 | 1:A:133:ILE:H    | 2        | 0.77          |
| (1,723) | 1:A:133:ILE:HG22 | 1:A:133:ILE:H    | 2        | 0.77          |
| (1,723) | 1:A:133:ILE:HG23 | 1:A:133:ILE:H    | 2        | 0.77          |
| (1,717) | 1:A:133:ILE:HG21 | 1:A:132:THR:H    | 8        | 0.77          |
| (1,717) | 1:A:133:ILE:HG22 | 1:A:132:THR:H    | 8        | 0.77          |
| (1,717) | 1:A:133:ILE:HG23 | 1:A:132:THR:H    | 8        | 0.77          |
| (1,714) | 1:A:133:ILE:HD11 | 1:A:130:PRO:HA   | 7        | 0.77          |
| (1,714) | 1:A:133:ILE:HD12 | 1:A:130:PRO:HA   | 7        | 0.77          |
| (1,714) | 1:A:133:ILE:HD13 | 1:A:130:PRO:HA   | 7        | 0.77          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD11 | 3        | 0.77          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD12 | 3        | 0.77          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD13 | 3        | 0.77          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD11 | 3        | 0.77          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD12 | 3        | 0.77          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD13 | 3        | 0.77          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD11 | 3        | 0.77          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD12 | 3        | 0.77          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD13 | 3        | 0.77          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD11 | 7        | 0.77          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD12 | 7        | 0.77          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD13 | 7        | 0.77          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD11 | 7        | 0.77          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD12 | 7        | 0.77          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD13 | 7        | 0.77          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD11 | 7        | 0.77          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD12 | 7        | 0.77          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD13 | 7        | 0.77          |
| (1,624) | 1:A:124:ILE:HB   | 1:A:124:ILE:HD11 | 6        | 0.77          |
| (1,624) | 1:A:124:ILE:HB   | 1:A:124:ILE:HD12 | 6        | 0.77          |
| (1,624) | 1:A:124:ILE:HB   | 1:A:124:ILE:HD13 | 6        | 0.77          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG11  | 4        | 0.77          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG12  | 4        | 0.77          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG13  | 4        | 0.77          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG21  | 4        | 0.77          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG22  | 4        | 0.77          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG23  | 4        | 0.77          |
| (1,579) | 1:A:119:HIS:H    | 1:A:120:ARG:H    | 3        | 0.77          |
| (1,559) | 1:A:118:PHE:HA   | 1:A:118:PHE:HD1  | 3        | 0.77          |
| (1,559) | 1:A:118:PHE:HA   | 1:A:118:PHE:HD2  | 3        | 0.77          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,511)  | 1:A:114:ILE:HG21 | 1:A:112:GLY:H    | 7        | 0.77          |
| (1,511)  | 1:A:114:ILE:HG22 | 1:A:112:GLY:H    | 7        | 0.77          |
| (1,511)  | 1:A:114:ILE:HG23 | 1:A:112:GLY:H    | 7        | 0.77          |
| (1,459)  | 1:A:111:HIS:H    | 1:A:110:GLU:H    | 3        | 0.77          |
| (1,458)  | 1:A:111:HIS:H    | 1:A:110:GLU:H    | 3        | 0.77          |
| (1,449)  | 1:A:109:ASP:HA   | 1:A:111:HIS:H    | 8        | 0.77          |
| (1,381)  | 1:A:101:HIS:HA   | 1:A:102:GLY:H    | 1        | 0.77          |
| (1,200)  | 1:A:84:PHE:HD1   | 1:A:85:SER:H     | 1        | 0.77          |
| (1,200)  | 1:A:84:PHE:HD2   | 1:A:85:SER:H     | 1        | 0.77          |
| (1,1762) | 1:A:122:TYR:HB2  | 1:B:111:HIS:H    | 4        | 0.77          |
| (1,1762) | 1:A:122:TYR:HB3  | 1:B:111:HIS:H    | 4        | 0.77          |
| (1,1611) | 1:B:135:SER:HB3  | 1:B:146:ASP:H    | 1        | 0.77          |
| (1,1584) | 1:B:133:ILE:HG21 | 1:B:132:THR:H    | 8        | 0.77          |
| (1,1584) | 1:B:133:ILE:HG22 | 1:B:132:THR:H    | 8        | 0.77          |
| (1,1584) | 1:B:133:ILE:HG23 | 1:B:132:THR:H    | 8        | 0.77          |
| (1,1581) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HA   | 7        | 0.77          |
| (1,1581) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HA   | 7        | 0.77          |
| (1,1581) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HA   | 7        | 0.77          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD11 | 4        | 0.77          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD12 | 4        | 0.77          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD13 | 4        | 0.77          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD11 | 4        | 0.77          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD12 | 4        | 0.77          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD13 | 4        | 0.77          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD11 | 6        | 0.77          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD12 | 6        | 0.77          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD13 | 6        | 0.77          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG11  | 4        | 0.77          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG12  | 4        | 0.77          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG13  | 4        | 0.77          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG21  | 4        | 0.77          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG22  | 4        | 0.77          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG23  | 4        | 0.77          |
| (1,1446) | 1:B:119:HIS:H    | 1:B:120:ARG:H    | 3        | 0.77          |
| (1,1426) | 1:B:118:PHE:HA   | 1:B:118:PHE:HD1  | 3        | 0.77          |
| (1,1426) | 1:B:118:PHE:HA   | 1:B:118:PHE:HD2  | 3        | 0.77          |
| (1,1378) | 1:B:114:ILE:HG21 | 1:B:112:GLY:H    | 7        | 0.77          |
| (1,1378) | 1:B:114:ILE:HG22 | 1:B:112:GLY:H    | 7        | 0.77          |
| (1,1378) | 1:B:114:ILE:HG23 | 1:B:112:GLY:H    | 7        | 0.77          |
| (1,1326) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 3        | 0.77          |
| (1,1325) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 3        | 0.77          |
| (1,1316) | 1:B:109:ASP:HA   | 1:B:111:HIS:H    | 8        | 0.77          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1248) | 1:B:101:HIS:HA   | 1:B:102:GLY:H   | 1        | 0.77          |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG2  | 3        | 0.77          |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG3  | 3        | 0.77          |
| (1,1067) | 1:B:84:PHE:HD1   | 1:B:85:SER:H    | 1        | 0.77          |
| (1,1067) | 1:B:84:PHE:HD2   | 1:B:85:SER:H    | 1        | 0.77          |
| (1,975)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:H    | 2        | 0.76          |
| (1,975)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:H    | 2        | 0.76          |
| (1,975)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:H    | 2        | 0.76          |
| (1,974)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HG   | 2        | 0.76          |
| (1,974)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HG   | 2        | 0.76          |
| (1,974)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HG   | 2        | 0.76          |
| (1,953)  | 1:B:77:VAL:HG21  | 1:B:75:PHE:HZ   | 9        | 0.76          |
| (1,953)  | 1:B:77:VAL:HG22  | 1:B:75:PHE:HZ   | 9        | 0.76          |
| (1,953)  | 1:B:77:VAL:HG23  | 1:B:75:PHE:HZ   | 9        | 0.76          |
| (1,95)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21 | 6        | 0.76          |
| (1,95)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22 | 6        | 0.76          |
| (1,95)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23 | 6        | 0.76          |
| (1,91)   | 1:A:77:VAL:HG11  | 1:A:77:VAL:HB   | 8        | 0.76          |
| (1,91)   | 1:A:77:VAL:HG12  | 1:A:77:VAL:HB   | 8        | 0.76          |
| (1,91)   | 1:A:77:VAL:HG13  | 1:A:77:VAL:HB   | 8        | 0.76          |
| (1,908)  | 1:B:74:ARG:HG2   | 1:B:74:ARG:H    | 5        | 0.76          |
| (1,908)  | 1:B:74:ARG:HG3   | 1:B:74:ARG:H    | 5        | 0.76          |
| (1,902)  | 1:B:73:ASP:H     | 1:B:74:ARG:HB3  | 9        | 0.76          |
| (1,89)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21 | 6        | 0.76          |
| (1,89)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22 | 6        | 0.76          |
| (1,89)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23 | 6        | 0.76          |
| (1,857)  | 1:A:150:LYS:H    | 1:A:150:LYS:HD2 | 7        | 0.76          |
| (1,857)  | 1:A:150:LYS:H    | 1:A:150:LYS:HD3 | 7        | 0.76          |
| (1,819)  | 1:A:145:VAL:HG21 | 1:A:145:VAL:H   | 6        | 0.76          |
| (1,819)  | 1:A:145:VAL:HG22 | 1:A:145:VAL:H   | 6        | 0.76          |
| (1,819)  | 1:A:145:VAL:HG23 | 1:A:145:VAL:H   | 6        | 0.76          |
| (1,558)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HZ  | 1        | 0.76          |
| (1,558)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HZ  | 2        | 0.76          |
| (1,459)  | 1:A:111:HIS:H    | 1:A:110:GLU:H   | 9        | 0.76          |
| (1,458)  | 1:A:111:HIS:H    | 1:A:110:GLU:H   | 9        | 0.76          |
| (1,41)   | 1:A:74:ARG:HG2   | 1:A:74:ARG:H    | 5        | 0.76          |
| (1,41)   | 1:A:74:ARG:HG3   | 1:A:74:ARG:H    | 5        | 0.76          |
| (1,35)   | 1:A:73:ASP:H     | 1:A:74:ARG:HB3  | 9        | 0.76          |
| (1,256)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2 | 7        | 0.76          |
| (1,255)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2 | 7        | 0.76          |
| (1,254)  | 1:A:89:LEU:HD11  | 1:A:91:VAL:HB   | 8        | 0.76          |
| (1,254)  | 1:A:89:LEU:HD12  | 1:A:91:VAL:HB   | 8        | 0.76          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,254)  | 1:A:89:LEU:HD13  | 1:A:91:VAL:HB    | 8        | 0.76          |
| (1,243)  | 1:A:89:LEU:HD11  | 1:A:88:GLU:H     | 6        | 0.76          |
| (1,243)  | 1:A:89:LEU:HD12  | 1:A:88:GLU:H     | 6        | 0.76          |
| (1,243)  | 1:A:89:LEU:HD13  | 1:A:88:GLU:H     | 6        | 0.76          |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG2   | 3        | 0.76          |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG3   | 3        | 0.76          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD2  | 7        | 0.76          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD3  | 7        | 0.76          |
| (1,1712) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HD11 | 2        | 0.76          |
| (1,1712) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HD12 | 2        | 0.76          |
| (1,1712) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HD13 | 2        | 0.76          |
| (1,1686) | 1:B:145:VAL:HG21 | 1:B:145:VAL:H    | 6        | 0.76          |
| (1,1686) | 1:B:145:VAL:HG22 | 1:B:145:VAL:H    | 6        | 0.76          |
| (1,1686) | 1:B:145:VAL:HG23 | 1:B:145:VAL:H    | 6        | 0.76          |
| (1,1590) | 1:B:133:ILE:HG21 | 1:B:133:ILE:H    | 2        | 0.76          |
| (1,1590) | 1:B:133:ILE:HG22 | 1:B:133:ILE:H    | 2        | 0.76          |
| (1,1590) | 1:B:133:ILE:HG23 | 1:B:133:ILE:H    | 2        | 0.76          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD11 | 5        | 0.76          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD12 | 5        | 0.76          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD13 | 5        | 0.76          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD11 | 5        | 0.76          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD12 | 5        | 0.76          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD13 | 5        | 0.76          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD11 | 5        | 0.76          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD12 | 5        | 0.76          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD13 | 5        | 0.76          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD11 | 4        | 0.76          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD12 | 4        | 0.76          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD13 | 4        | 0.76          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD11 | 8        | 0.76          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD12 | 8        | 0.76          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD13 | 8        | 0.76          |
| (1,143)  | 1:A:79:LEU:HG    | 1:A:80:ASP:H     | 6        | 0.76          |
| (1,1425) | 1:B:118:PHE:HA   | 1:B:118:PHE:HZ   | 1        | 0.76          |
| (1,1326) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 9        | 0.76          |
| (1,1325) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 9        | 0.76          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG21  | 5        | 0.76          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG22  | 5        | 0.76          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG23  | 5        | 0.76          |
| (1,1121) | 1:B:89:LEU:HD11  | 1:B:91:VAL:HB    | 8        | 0.76          |
| (1,1121) | 1:B:89:LEU:HD12  | 1:B:91:VAL:HB    | 8        | 0.76          |
| (1,1121) | 1:B:89:LEU:HD13  | 1:B:91:VAL:HB    | 8        | 0.76          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1110) | 1:B:89:LEU:HD11  | 1:B:88:GLU:H     | 6        | 0.76          |
| (1,1110) | 1:B:89:LEU:HD12  | 1:B:88:GLU:H     | 6        | 0.76          |
| (1,1110) | 1:B:89:LEU:HD13  | 1:B:88:GLU:H     | 6        | 0.76          |
| (1,108)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:H     | 2        | 0.76          |
| (1,108)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:H     | 2        | 0.76          |
| (1,108)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:H     | 2        | 0.76          |
| (1,107)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:HG    | 2        | 0.76          |
| (1,107)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:HG    | 2        | 0.76          |
| (1,107)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:HG    | 2        | 0.76          |
| (1,1010) | 1:B:79:LEU:HG    | 1:B:80:ASP:H     | 6        | 0.76          |
| (1,973)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HB2   | 5        | 0.75          |
| (1,973)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HB3   | 5        | 0.75          |
| (1,973)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HB2   | 5        | 0.75          |
| (1,973)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HB3   | 5        | 0.75          |
| (1,973)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HB2   | 5        | 0.75          |
| (1,973)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HB3   | 5        | 0.75          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG2   | 1        | 0.75          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG3   | 1        | 0.75          |
| (1,861)  | 1:A:150:LYS:HA   | 1:A:151:GLN:H    | 4        | 0.75          |
| (1,703)  | 1:A:132:THR:HA   | 1:A:133:ILE:HA   | 2        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD11 | 2        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD12 | 2        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD13 | 2        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD11 | 2        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD12 | 2        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD13 | 2        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD11 | 8        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD12 | 8        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD13 | 8        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD11 | 8        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD12 | 8        | 0.75          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD13 | 8        | 0.75          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD11 | 5        | 0.75          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD12 | 5        | 0.75          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD13 | 5        | 0.75          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD11 | 5        | 0.75          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD12 | 5        | 0.75          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD13 | 5        | 0.75          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD11 | 5        | 0.75          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD12 | 5        | 0.75          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD13 | 5        | 0.75          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD11 | 4        | 0.75          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD12 | 4        | 0.75          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD13 | 4        | 0.75          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD11 | 8        | 0.75          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD12 | 8        | 0.75          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD13 | 8        | 0.75          |
| (1,583)  | 1:A:121:LYS:HA   | 1:A:99:GLU:HA    | 1        | 0.75          |
| (1,582)  | 1:A:121:LYS:HA   | 1:A:97:VAL:HG11  | 6        | 0.75          |
| (1,582)  | 1:A:121:LYS:HA   | 1:A:97:VAL:HG12  | 6        | 0.75          |
| (1,582)  | 1:A:121:LYS:HA   | 1:A:97:VAL:HG13  | 6        | 0.75          |
| (1,582)  | 1:A:121:LYS:HA   | 1:A:97:VAL:HG21  | 6        | 0.75          |
| (1,582)  | 1:A:121:LYS:HA   | 1:A:97:VAL:HG22  | 6        | 0.75          |
| (1,582)  | 1:A:121:LYS:HA   | 1:A:97:VAL:HG23  | 6        | 0.75          |
| (1,544)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 1        | 0.75          |
| (1,543)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 1        | 0.75          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB2  | 6        | 0.75          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB3  | 6        | 0.75          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB2  | 9        | 0.75          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB3  | 9        | 0.75          |
| (1,358)  | 1:A:100:VAL:HG11 | 1:A:92:LYS:H     | 8        | 0.75          |
| (1,358)  | 1:A:100:VAL:HG12 | 1:A:92:LYS:H     | 8        | 0.75          |
| (1,358)  | 1:A:100:VAL:HG13 | 1:A:92:LYS:H     | 8        | 0.75          |
| (1,296)  | 1:A:94:LEU:H     | 1:A:99:GLU:H     | 2        | 0.75          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG21  | 5        | 0.75          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG22  | 5        | 0.75          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG23  | 5        | 0.75          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG2   | 1        | 0.75          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG3   | 1        | 0.75          |
| (1,190)  | 1:A:84:PHE:HE1   | 1:A:82:LYS:H     | 6        | 0.75          |
| (1,190)  | 1:A:84:PHE:HE2   | 1:A:82:LYS:H     | 6        | 0.75          |
| (1,1570) | 1:B:132:THR:HA   | 1:B:133:ILE:HA   | 2        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD11 | 2        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD12 | 2        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD13 | 2        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD11 | 2        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD12 | 2        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD13 | 2        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD11 | 8        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD12 | 8        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD13 | 8        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD11 | 8        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD12 | 8        | 0.75          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD13 | 8        | 0.75          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1450) | 1:B:121:LYS:HA   | 1:B:99:GLU:HA   | 1        | 0.75          |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG11 | 6        | 0.75          |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG12 | 6        | 0.75          |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG13 | 6        | 0.75          |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG21 | 6        | 0.75          |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG22 | 6        | 0.75          |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG23 | 6        | 0.75          |
| (1,1425) | 1:B:118:PHE:HA   | 1:B:118:PHE:HZ  | 2        | 0.75          |
| (1,1411) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA  | 1        | 0.75          |
| (1,1410) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA  | 1        | 0.75          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB2 | 6        | 0.75          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB3 | 6        | 0.75          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB2 | 9        | 0.75          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB3 | 9        | 0.75          |
| (1,1225) | 1:B:100:VAL:HG11 | 1:B:92:LYS:H    | 8        | 0.75          |
| (1,1225) | 1:B:100:VAL:HG12 | 1:B:92:LYS:H    | 8        | 0.75          |
| (1,1225) | 1:B:100:VAL:HG13 | 1:B:92:LYS:H    | 8        | 0.75          |
| (1,1163) | 1:B:94:LEU:H     | 1:B:99:GLU:H    | 2        | 0.75          |
| (1,1123) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2 | 7        | 0.75          |
| (1,1122) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2 | 7        | 0.75          |
| (1,106)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:HB2  | 5        | 0.75          |
| (1,106)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:HB3  | 5        | 0.75          |
| (1,106)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:HB2  | 5        | 0.75          |
| (1,106)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:HB3  | 5        | 0.75          |
| (1,106)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:HB2  | 5        | 0.75          |
| (1,106)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:HB3  | 5        | 0.75          |
| (1,1057) | 1:B:84:PHE:HE1   | 1:B:82:LYS:H    | 6        | 0.75          |
| (1,1057) | 1:B:84:PHE:HE2   | 1:B:82:LYS:H    | 6        | 0.75          |
| (1,975)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:H    | 4        | 0.74          |
| (1,975)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:H    | 4        | 0.74          |
| (1,975)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:H    | 4        | 0.74          |
| (1,969)  | 1:B:77:VAL:HG11  | 1:B:78:ASN:H    | 2        | 0.74          |
| (1,969)  | 1:B:77:VAL:HG12  | 1:B:78:ASN:H    | 2        | 0.74          |
| (1,969)  | 1:B:77:VAL:HG13  | 1:B:78:ASN:H    | 2        | 0.74          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21 | 9        | 0.74          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22 | 9        | 0.74          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23 | 9        | 0.74          |
| (1,956)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21 | 9        | 0.74          |
| (1,956)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22 | 9        | 0.74          |
| (1,956)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23 | 9        | 0.74          |
| (1,95)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21 | 9        | 0.74          |
| (1,95)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22 | 9        | 0.74          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 9        | 0.74          |
| (1,917) | 1:B:75:PHE:HD1   | 1:B:75:PHE:H     | 2        | 0.74          |
| (1,917) | 1:B:75:PHE:HD2   | 1:B:75:PHE:H     | 2        | 0.74          |
| (1,908) | 1:B:74:ARG:HG2   | 1:B:74:ARG:H     | 7        | 0.74          |
| (1,908) | 1:B:74:ARG:HG3   | 1:B:74:ARG:H     | 7        | 0.74          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 9        | 0.74          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 9        | 0.74          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 9        | 0.74          |
| (1,880) | 1:B:68:MET:HE1   | 1:B:122:TYR:HE1  | 3        | 0.74          |
| (1,880) | 1:B:68:MET:HE1   | 1:B:122:TYR:HE2  | 3        | 0.74          |
| (1,880) | 1:B:68:MET:HE2   | 1:B:122:TYR:HE1  | 3        | 0.74          |
| (1,880) | 1:B:68:MET:HE2   | 1:B:122:TYR:HE2  | 3        | 0.74          |
| (1,880) | 1:B:68:MET:HE3   | 1:B:122:TYR:HE1  | 3        | 0.74          |
| (1,880) | 1:B:68:MET:HE3   | 1:B:122:TYR:HE2  | 3        | 0.74          |
| (1,855) | 1:A:149:ARG:HB2  | 1:A:149:ARG:H    | 5        | 0.74          |
| (1,855) | 1:A:149:ARG:HB3  | 1:A:149:ARG:H    | 5        | 0.74          |
| (1,845) | 1:A:147:GLY:HA2  | 1:A:133:ILE:HD11 | 2        | 0.74          |
| (1,845) | 1:A:147:GLY:HA2  | 1:A:133:ILE:HD12 | 2        | 0.74          |
| (1,845) | 1:A:147:GLY:HA2  | 1:A:133:ILE:HD13 | 2        | 0.74          |
| (1,758) | 1:A:138:SER:HA   | 1:A:141:GLY:H    | 9        | 0.74          |
| (1,703) | 1:A:132:THR:HA   | 1:A:133:ILE:HA   | 4        | 0.74          |
| (1,699) | 1:A:132:THR:HG1  | 1:A:132:THR:H    | 6        | 0.74          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD11 | 1        | 0.74          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD12 | 1        | 0.74          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD13 | 1        | 0.74          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD11 | 1        | 0.74          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD12 | 1        | 0.74          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD13 | 1        | 0.74          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD11 | 3        | 0.74          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD12 | 3        | 0.74          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD13 | 3        | 0.74          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD11 | 3        | 0.74          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD12 | 3        | 0.74          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD13 | 3        | 0.74          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD11 | 5        | 0.74          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD12 | 5        | 0.74          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD13 | 5        | 0.74          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD11 | 5        | 0.74          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD12 | 5        | 0.74          |
| (1,627) | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD13 | 5        | 0.74          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD11 | 6        | 0.74          |
| (1,627) | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD12 | 6        | 0.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD13 | 6        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD11 | 6        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD12 | 6        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD13 | 6        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD11 | 7        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD12 | 7        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD13 | 7        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD11 | 7        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD12 | 7        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD13 | 7        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD11 | 9        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD12 | 9        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG12 | 1:A:124:ILE:HD13 | 9        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD11 | 9        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD12 | 9        | 0.74          |
| (1,627)  | 1:A:124:ILE:HG13 | 1:A:124:ILE:HD13 | 9        | 0.74          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD11 | 9        | 0.74          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD12 | 9        | 0.74          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD13 | 9        | 0.74          |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB2  | 3        | 0.74          |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB3  | 3        | 0.74          |
| (1,506)  | 1:A:114:ILE:HB   | 1:A:107:ARG:HD3  | 1        | 0.74          |
| (1,50)   | 1:A:75:PHE:HD1   | 1:A:75:PHE:H     | 2        | 0.74          |
| (1,50)   | 1:A:75:PHE:HD2   | 1:A:75:PHE:H     | 2        | 0.74          |
| (1,445)  | 1:A:108:GLN:HA   | 1:A:113:PHE:H    | 6        | 0.74          |
| (1,41)   | 1:A:74:ARG:HG2   | 1:A:74:ARG:H     | 7        | 0.74          |
| (1,41)   | 1:A:74:ARG:HG3   | 1:A:74:ARG:H     | 7        | 0.74          |
| (1,236)  | 1:A:89:LEU:HD21  | 1:A:85:SER:HB3   | 2        | 0.74          |
| (1,236)  | 1:A:89:LEU:HD22  | 1:A:85:SER:HB3   | 2        | 0.74          |
| (1,236)  | 1:A:89:LEU:HD23  | 1:A:85:SER:HB3   | 2        | 0.74          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB2   | 9        | 0.74          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB3   | 9        | 0.74          |
| (1,1768) | 1:A:122:TYR:HA   | 1:B:112:GLY:H    | 1        | 0.74          |
| (1,1743) | 1:A:114:ILE:HG21 | 1:B:119:HIS:H    | 5        | 0.74          |
| (1,1743) | 1:A:114:ILE:HG22 | 1:B:119:HIS:H    | 5        | 0.74          |
| (1,1743) | 1:A:114:ILE:HG23 | 1:B:119:HIS:H    | 5        | 0.74          |
| (1,1728) | 1:B:150:LYS:HA   | 1:B:151:GLN:H    | 4        | 0.74          |
| (1,1722) | 1:B:149:ARG:HB2  | 1:B:149:ARG:H    | 5        | 0.74          |
| (1,1722) | 1:B:149:ARG:HB3  | 1:B:149:ARG:H    | 5        | 0.74          |
| (1,1625) | 1:B:138:SER:HA   | 1:B:141:GLY:H    | 9        | 0.74          |
| (1,1570) | 1:B:132:THR:HA   | 1:B:133:ILE:HA   | 4        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD11 | 1        | 0.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD12 | 1        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD13 | 1        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD11 | 1        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD12 | 1        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD13 | 1        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD11 | 3        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD12 | 3        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD13 | 3        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD11 | 3        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD12 | 3        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD13 | 3        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD11 | 5        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD12 | 5        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD13 | 5        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD11 | 5        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD12 | 5        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD13 | 5        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD11 | 6        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD12 | 6        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD13 | 6        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD11 | 6        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD12 | 6        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD13 | 6        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD11 | 7        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD12 | 7        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD13 | 7        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD11 | 7        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD12 | 7        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD13 | 7        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD11 | 9        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD12 | 9        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG12 | 1:B:124:ILE:HD13 | 9        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD11 | 9        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD12 | 9        | 0.74          |
| (1,1494) | 1:B:124:ILE:HG13 | 1:B:124:ILE:HD13 | 9        | 0.74          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD11 | 2        | 0.74          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD12 | 2        | 0.74          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD13 | 2        | 0.74          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD11 | 2        | 0.74          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD12 | 2        | 0.74          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD13 | 2        | 0.74          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD11 | 2        | 0.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD12 | 2        | 0.74          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD13 | 2        | 0.74          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD11 | 9        | 0.74          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD12 | 9        | 0.74          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD13 | 9        | 0.74          |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB2  | 3        | 0.74          |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB3  | 3        | 0.74          |
| (1,1373) | 1:B:114:ILE:HB   | 1:B:107:ARG:HD3  | 1        | 0.74          |
| (1,1312) | 1:B:108:GLN:HA   | 1:B:113:PHE:H    | 6        | 0.74          |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE1  | 3        | 0.74          |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE2  | 3        | 0.74          |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE1  | 3        | 0.74          |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE2  | 3        | 0.74          |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE1  | 3        | 0.74          |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE2  | 3        | 0.74          |
| (1,1103) | 1:B:89:LEU:HD21  | 1:B:85:SER:HB3   | 2        | 0.74          |
| (1,1103) | 1:B:89:LEU:HD22  | 1:B:85:SER:HB3   | 2        | 0.74          |
| (1,1103) | 1:B:89:LEU:HD23  | 1:B:85:SER:HB3   | 2        | 0.74          |
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB2   | 9        | 0.74          |
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB3   | 9        | 0.74          |
| (1,108)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:H     | 4        | 0.74          |
| (1,108)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:H     | 4        | 0.74          |
| (1,108)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:H     | 4        | 0.74          |
| (1,102)  | 1:A:77:VAL:HG11  | 1:A:78:ASN:H     | 2        | 0.74          |
| (1,102)  | 1:A:77:VAL:HG12  | 1:A:78:ASN:H     | 2        | 0.74          |
| (1,102)  | 1:A:77:VAL:HG13  | 1:A:78:ASN:H     | 2        | 0.74          |
| (1,977)  | 1:B:77:VAL:HG11  | 1:B:98:ILE:HD11  | 6        | 0.73          |
| (1,977)  | 1:B:77:VAL:HG11  | 1:B:98:ILE:HD12  | 6        | 0.73          |
| (1,977)  | 1:B:77:VAL:HG11  | 1:B:98:ILE:HD13  | 6        | 0.73          |
| (1,977)  | 1:B:77:VAL:HG12  | 1:B:98:ILE:HD11  | 6        | 0.73          |
| (1,977)  | 1:B:77:VAL:HG12  | 1:B:98:ILE:HD12  | 6        | 0.73          |
| (1,977)  | 1:B:77:VAL:HG12  | 1:B:98:ILE:HD13  | 6        | 0.73          |
| (1,977)  | 1:B:77:VAL:HG13  | 1:B:98:ILE:HD11  | 6        | 0.73          |
| (1,977)  | 1:B:77:VAL:HG13  | 1:B:98:ILE:HD12  | 6        | 0.73          |
| (1,977)  | 1:B:77:VAL:HG13  | 1:B:98:ILE:HD13  | 6        | 0.73          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 1        | 0.73          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 1        | 0.73          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 1        | 0.73          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 5        | 0.73          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 5        | 0.73          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 5        | 0.73          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 7        | 0.73          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,962) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 7        | 0.73          |
| (1,962) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 7        | 0.73          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 1        | 0.73          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 1        | 0.73          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 1        | 0.73          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 5        | 0.73          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 5        | 0.73          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 5        | 0.73          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 7        | 0.73          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 7        | 0.73          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 7        | 0.73          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 1        | 0.73          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 1        | 0.73          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 1        | 0.73          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 5        | 0.73          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 5        | 0.73          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 5        | 0.73          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 7        | 0.73          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 7        | 0.73          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 7        | 0.73          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 1        | 0.73          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 1        | 0.73          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 1        | 0.73          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 5        | 0.73          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 5        | 0.73          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 5        | 0.73          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 7        | 0.73          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 7        | 0.73          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 7        | 0.73          |
| (1,887) | 1:B:70:LEU:HB3   | 1:B:71:GLU:H     | 8        | 0.73          |
| (1,723) | 1:A:133:ILE:HG21 | 1:A:133:ILE:H    | 3        | 0.73          |
| (1,723) | 1:A:133:ILE:HG22 | 1:A:133:ILE:H    | 3        | 0.73          |
| (1,723) | 1:A:133:ILE:HG23 | 1:A:133:ILE:H    | 3        | 0.73          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD11 | 2        | 0.73          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD12 | 2        | 0.73          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD13 | 2        | 0.73          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD11 | 2        | 0.73          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD12 | 2        | 0.73          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD13 | 2        | 0.73          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD11 | 2        | 0.73          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD12 | 2        | 0.73          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD13 | 2        | 0.73          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,566)  | 1:A:118:PHE:HA   | 1:A:119:HIS:H    | 2        | 0.73          |
| (1,558)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HZ   | 6        | 0.73          |
| (1,480)  | 1:A:112:GLY:HA3  | 1:A:113:PHE:H    | 7        | 0.73          |
| (1,459)  | 1:A:111:HIS:H    | 1:A:110:GLU:H    | 1        | 0.73          |
| (1,458)  | 1:A:111:HIS:H    | 1:A:110:GLU:H    | 1        | 0.73          |
| (1,449)  | 1:A:109:ASP:HA   | 1:A:111:HIS:H    | 4        | 0.73          |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG21 | 9        | 0.73          |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG22 | 9        | 0.73          |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG23 | 9        | 0.73          |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG21 | 9        | 0.73          |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG22 | 9        | 0.73          |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG23 | 9        | 0.73          |
| (1,321)  | 1:A:97:VAL:H     | 1:A:93:VAL:HB    | 7        | 0.73          |
| (1,20)   | 1:A:70:LEU:HB3   | 1:A:71:GLU:H     | 8        | 0.73          |
| (1,1590) | 1:B:133:ILE:HG21 | 1:B:133:ILE:H    | 3        | 0.73          |
| (1,1590) | 1:B:133:ILE:HG22 | 1:B:133:ILE:H    | 3        | 0.73          |
| (1,1590) | 1:B:133:ILE:HG23 | 1:B:133:ILE:H    | 3        | 0.73          |
| (1,1499) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 5        | 0.73          |
| (1,1499) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 5        | 0.73          |
| (1,1499) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 5        | 0.73          |
| (1,1498) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 5        | 0.73          |
| (1,1498) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 5        | 0.73          |
| (1,1498) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 5        | 0.73          |
| (1,1433) | 1:B:118:PHE:HA   | 1:B:119:HIS:H    | 2        | 0.73          |
| (1,1347) | 1:B:112:GLY:HA3  | 1:B:113:PHE:H    | 7        | 0.73          |
| (1,1326) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 1        | 0.73          |
| (1,1325) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 1        | 0.73          |
| (1,1316) | 1:B:109:ASP:HA   | 1:B:111:HIS:H    | 4        | 0.73          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG21 | 9        | 0.73          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG22 | 9        | 0.73          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG23 | 9        | 0.73          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG21 | 9        | 0.73          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG22 | 9        | 0.73          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG23 | 9        | 0.73          |
| (1,1188) | 1:B:97:VAL:H     | 1:B:93:VAL:HB    | 7        | 0.73          |
| (1,110)  | 1:A:77:VAL:HG11  | 1:A:98:ILE:HD11  | 6        | 0.73          |
| (1,110)  | 1:A:77:VAL:HG11  | 1:A:98:ILE:HD12  | 6        | 0.73          |
| (1,110)  | 1:A:77:VAL:HG11  | 1:A:98:ILE:HD13  | 6        | 0.73          |
| (1,110)  | 1:A:77:VAL:HG12  | 1:A:98:ILE:HD11  | 6        | 0.73          |
| (1,110)  | 1:A:77:VAL:HG12  | 1:A:98:ILE:HD12  | 6        | 0.73          |
| (1,110)  | 1:A:77:VAL:HG12  | 1:A:98:ILE:HD13  | 6        | 0.73          |
| (1,110)  | 1:A:77:VAL:HG13  | 1:A:98:ILE:HD11  | 6        | 0.73          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,110) | 1:A:77:VAL:HG13  | 1:A:98:ILE:HD12  | 6        | 0.73          |
| (1,110) | 1:A:77:VAL:HG13  | 1:A:98:ILE:HD13  | 6        | 0.73          |
| (1,920) | 1:B:75:PHE:HE1   | 1:B:133:ILE:HD11 | 6        | 0.72          |
| (1,920) | 1:B:75:PHE:HE1   | 1:B:133:ILE:HD12 | 6        | 0.72          |
| (1,920) | 1:B:75:PHE:HE1   | 1:B:133:ILE:HD13 | 6        | 0.72          |
| (1,920) | 1:B:75:PHE:HE2   | 1:B:133:ILE:HD11 | 6        | 0.72          |
| (1,920) | 1:B:75:PHE:HE2   | 1:B:133:ILE:HD12 | 6        | 0.72          |
| (1,920) | 1:B:75:PHE:HE2   | 1:B:133:ILE:HD13 | 6        | 0.72          |
| (1,86)  | 1:A:77:VAL:HG21  | 1:A:75:PHE:HZ    | 9        | 0.72          |
| (1,86)  | 1:A:77:VAL:HG22  | 1:A:75:PHE:HZ    | 9        | 0.72          |
| (1,86)  | 1:A:77:VAL:HG23  | 1:A:75:PHE:HZ    | 9        | 0.72          |
| (1,831) | 1:A:146:ASP:HB2  | 1:A:145:VAL:HA   | 2        | 0.72          |
| (1,758) | 1:A:138:SER:HA   | 1:A:141:GLY:H    | 1        | 0.72          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG21 | 8        | 0.72          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG22 | 8        | 0.72          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG23 | 8        | 0.72          |
| (1,703) | 1:A:132:THR:HA   | 1:A:133:ILE:HA   | 3        | 0.72          |
| (1,642) | 1:A:125:PRO:HD3  | 1:A:122:TYR:HD1  | 9        | 0.72          |
| (1,642) | 1:A:125:PRO:HD3  | 1:A:122:TYR:HD2  | 9        | 0.72          |
| (1,632) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 5        | 0.72          |
| (1,632) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 5        | 0.72          |
| (1,632) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 5        | 0.72          |
| (1,631) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 5        | 0.72          |
| (1,631) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 5        | 0.72          |
| (1,631) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 5        | 0.72          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD11 | 9        | 0.72          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD12 | 9        | 0.72          |
| (1,625) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD13 | 9        | 0.72          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD11 | 9        | 0.72          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD12 | 9        | 0.72          |
| (1,625) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD13 | 9        | 0.72          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD11 | 9        | 0.72          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD12 | 9        | 0.72          |
| (1,625) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD13 | 9        | 0.72          |
| (1,498) | 1:A:113:PHE:HB2  | 1:A:113:PHE:H    | 3        | 0.72          |
| (1,473) | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG21 | 4        | 0.72          |
| (1,473) | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG22 | 4        | 0.72          |
| (1,473) | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG23 | 4        | 0.72          |
| (1,409) | 1:A:104:HIS:H    | 1:A:116:ARG:HB2  | 9        | 0.72          |
| (1,409) | 1:A:104:HIS:H    | 1:A:116:ARG:HB3  | 9        | 0.72          |
| (1,397) | 1:A:103:LYS:HG2  | 1:A:116:ARG:H    | 8        | 0.72          |
| (1,397) | 1:A:103:LYS:HG3  | 1:A:116:ARG:H    | 8        | 0.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,288)  | 1:A:93:VAL:HA    | 1:A:99:GLU:H     | 2        | 0.72          |
| (1,1767) | 1:A:122:TYR:HB2  | 1:B:112:GLY:HA3  | 2        | 0.72          |
| (1,1767) | 1:A:122:TYR:HB3  | 1:B:112:GLY:HA3  | 2        | 0.72          |
| (1,1698) | 1:B:146:ASP:HB2  | 1:B:145:VAL:HA   | 2        | 0.72          |
| (1,1625) | 1:B:138:SER:HA   | 1:B:141:GLY:H    | 1        | 0.72          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG21 | 8        | 0.72          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG22 | 8        | 0.72          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG23 | 8        | 0.72          |
| (1,1509) | 1:B:125:PRO:HD3  | 1:B:122:TYR:HD1  | 9        | 0.72          |
| (1,1509) | 1:B:125:PRO:HD3  | 1:B:122:TYR:HD2  | 9        | 0.72          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD11 | 9        | 0.72          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD12 | 9        | 0.72          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD13 | 9        | 0.72          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD11 | 9        | 0.72          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD12 | 9        | 0.72          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD13 | 9        | 0.72          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD11 | 9        | 0.72          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD12 | 9        | 0.72          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD13 | 9        | 0.72          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD11 | 2        | 0.72          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD12 | 2        | 0.72          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD13 | 2        | 0.72          |
| (1,1425) | 1:B:118:PHE:HA   | 1:B:118:PHE:HZ   | 6        | 0.72          |
| (1,1365) | 1:B:113:PHE:HB2  | 1:B:113:PHE:H    | 3        | 0.72          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG21 | 4        | 0.72          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG22 | 4        | 0.72          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG23 | 4        | 0.72          |
| (1,1276) | 1:B:104:HIS:H    | 1:B:116:ARG:HB2  | 9        | 0.72          |
| (1,1276) | 1:B:104:HIS:H    | 1:B:116:ARG:HB3  | 9        | 0.72          |
| (1,1264) | 1:B:103:LYS:HG2  | 1:B:116:ARG:H    | 8        | 0.72          |
| (1,1264) | 1:B:103:LYS:HG3  | 1:B:116:ARG:H    | 8        | 0.72          |
| (1,1155) | 1:B:93:VAL:HA    | 1:B:99:GLU:H     | 2        | 0.72          |
| (1,908)  | 1:B:74:ARG:HG2   | 1:B:74:ARG:H     | 2        | 0.71          |
| (1,908)  | 1:B:74:ARG:HG3   | 1:B:74:ARG:H     | 2        | 0.71          |
| (1,841)  | 1:A:147:GLY:HA2  | 1:A:132:THR:HA   | 7        | 0.71          |
| (1,809)  | 1:A:144:THR:HG21 | 1:A:146:ASP:HB3  | 5        | 0.71          |
| (1,809)  | 1:A:144:THR:HG22 | 1:A:146:ASP:HB3  | 5        | 0.71          |
| (1,809)  | 1:A:144:THR:HG23 | 1:A:146:ASP:HB3  | 5        | 0.71          |
| (1,643)  | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD1  | 7        | 0.71          |
| (1,643)  | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD2  | 7        | 0.71          |
| (1,632)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 1        | 0.71          |
| (1,632)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 1        | 0.71          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,632) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 1        | 0.71          |
| (1,632) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 2        | 0.71          |
| (1,632) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 2        | 0.71          |
| (1,632) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 2        | 0.71          |
| (1,632) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 6        | 0.71          |
| (1,632) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 6        | 0.71          |
| (1,632) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 6        | 0.71          |
| (1,631) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 1        | 0.71          |
| (1,631) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 1        | 0.71          |
| (1,631) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 1        | 0.71          |
| (1,631) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 2        | 0.71          |
| (1,631) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 2        | 0.71          |
| (1,631) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 2        | 0.71          |
| (1,631) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 6        | 0.71          |
| (1,631) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 6        | 0.71          |
| (1,631) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 6        | 0.71          |
| (1,624) | 1:A:124:ILE:HB   | 1:A:124:ILE:HD11 | 2        | 0.71          |
| (1,624) | 1:A:124:ILE:HB   | 1:A:124:ILE:HD12 | 2        | 0.71          |
| (1,624) | 1:A:124:ILE:HB   | 1:A:124:ILE:HD13 | 2        | 0.71          |
| (1,624) | 1:A:124:ILE:HB   | 1:A:124:ILE:HD11 | 5        | 0.71          |
| (1,624) | 1:A:124:ILE:HB   | 1:A:124:ILE:HD12 | 5        | 0.71          |
| (1,624) | 1:A:124:ILE:HB   | 1:A:124:ILE:HD13 | 5        | 0.71          |
| (1,579) | 1:A:119:HIS:H    | 1:A:120:ARG:H    | 8        | 0.71          |
| (1,566) | 1:A:118:PHE:HA   | 1:A:119:HIS:H    | 7        | 0.71          |
| (1,53)  | 1:A:75:PHE:HE1   | 1:A:133:ILE:HD11 | 6        | 0.71          |
| (1,53)  | 1:A:75:PHE:HE1   | 1:A:133:ILE:HD12 | 6        | 0.71          |
| (1,53)  | 1:A:75:PHE:HE1   | 1:A:133:ILE:HD13 | 6        | 0.71          |
| (1,53)  | 1:A:75:PHE:HE2   | 1:A:133:ILE:HD11 | 6        | 0.71          |
| (1,53)  | 1:A:75:PHE:HE2   | 1:A:133:ILE:HD12 | 6        | 0.71          |
| (1,53)  | 1:A:75:PHE:HE2   | 1:A:133:ILE:HD13 | 6        | 0.71          |
| (1,432) | 1:A:107:ARG:HG2  | 1:A:108:GLN:H    | 4        | 0.71          |
| (1,432) | 1:A:107:ARG:HG3  | 1:A:108:GLN:H    | 4        | 0.71          |
| (1,41)  | 1:A:74:ARG:HG2   | 1:A:74:ARG:H     | 2        | 0.71          |
| (1,41)  | 1:A:74:ARG:HG3   | 1:A:74:ARG:H     | 2        | 0.71          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG21 | 1        | 0.71          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG22 | 1        | 0.71          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG23 | 1        | 0.71          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG21 | 1        | 0.71          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG22 | 1        | 0.71          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG23 | 1        | 0.71          |
| (1,256) | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2  | 2        | 0.71          |
| (1,255) | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2  | 2        | 0.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1767) | 1:A:122:TYR:HB2  | 1:B:112:GLY:HA3  | 3        | 0.71          |
| (1,1767) | 1:A:122:TYR:HB3  | 1:B:112:GLY:HA3  | 3        | 0.71          |
| (1,1708) | 1:B:147:GLY:HA2  | 1:B:132:THR:HA   | 7        | 0.71          |
| (1,1676) | 1:B:144:THR:HG21 | 1:B:146:ASP:HB3  | 5        | 0.71          |
| (1,1676) | 1:B:144:THR:HG22 | 1:B:146:ASP:HB3  | 5        | 0.71          |
| (1,1676) | 1:B:144:THR:HG23 | 1:B:146:ASP:HB3  | 5        | 0.71          |
| (1,1570) | 1:B:132:THR:HA   | 1:B:133:ILE:HA   | 3        | 0.71          |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD1  | 7        | 0.71          |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD2  | 7        | 0.71          |
| (1,1499) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 1        | 0.71          |
| (1,1499) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 1        | 0.71          |
| (1,1499) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 1        | 0.71          |
| (1,1499) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 6        | 0.71          |
| (1,1499) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 6        | 0.71          |
| (1,1499) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 6        | 0.71          |
| (1,1498) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 1        | 0.71          |
| (1,1498) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 1        | 0.71          |
| (1,1498) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 1        | 0.71          |
| (1,1498) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 6        | 0.71          |
| (1,1498) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 6        | 0.71          |
| (1,1498) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 6        | 0.71          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD11 | 5        | 0.71          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD12 | 5        | 0.71          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD13 | 5        | 0.71          |
| (1,149)  | 1:A:80:ASP:HA    | 1:A:81:VAL:H     | 7        | 0.71          |
| (1,149)  | 1:A:80:ASP:HA    | 1:A:81:VAL:H     | 9        | 0.71          |
| (1,1472) | 1:B:123:ARG:HD2  | 1:B:98:ILE:H     | 6        | 0.71          |
| (1,1472) | 1:B:123:ARG:HD3  | 1:B:98:ILE:H     | 6        | 0.71          |
| (1,1446) | 1:B:119:HIS:H    | 1:B:120:ARG:H    | 8        | 0.71          |
| (1,1433) | 1:B:118:PHE:HA   | 1:B:119:HIS:H    | 7        | 0.71          |
| (1,1299) | 1:B:107:ARG:HG2  | 1:B:108:GLN:H    | 4        | 0.71          |
| (1,1299) | 1:B:107:ARG:HG3  | 1:B:108:GLN:H    | 4        | 0.71          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG21 | 1        | 0.71          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG22 | 1        | 0.71          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG23 | 1        | 0.71          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG21 | 1        | 0.71          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG22 | 1        | 0.71          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG23 | 1        | 0.71          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD2   | 5        | 0.71          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD3   | 5        | 0.71          |
| (1,1123) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2  | 2        | 0.71          |
| (1,1122) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2  | 2        | 0.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1016) | 1:B:80:ASP:HA    | 1:B:81:VAL:H     | 7        | 0.71          |
| (1,1016) | 1:B:80:ASP:HA    | 1:B:81:VAL:H     | 9        | 0.71          |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG11  | 2        | 0.7           |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG12  | 2        | 0.7           |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG13  | 2        | 0.7           |
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG11  | 2        | 0.7           |
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG12  | 2        | 0.7           |
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG13  | 2        | 0.7           |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG11  | 2        | 0.7           |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG12  | 2        | 0.7           |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG13  | 2        | 0.7           |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG11  | 2        | 0.7           |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG12  | 2        | 0.7           |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG13  | 2        | 0.7           |
| (1,848)  | 1:A:147:GLY:HA3  | 1:A:147:GLY:H    | 8        | 0.7           |
| (1,819)  | 1:A:145:VAL:HG21 | 1:A:145:VAL:H    | 2        | 0.7           |
| (1,819)  | 1:A:145:VAL:HG22 | 1:A:145:VAL:H    | 2        | 0.7           |
| (1,819)  | 1:A:145:VAL:HG23 | 1:A:145:VAL:H    | 2        | 0.7           |
| (1,632)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 9        | 0.7           |
| (1,632)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 9        | 0.7           |
| (1,632)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 9        | 0.7           |
| (1,631)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 9        | 0.7           |
| (1,631)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 9        | 0.7           |
| (1,631)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 9        | 0.7           |
| (1,605)  | 1:A:123:ARG:HD2  | 1:A:98:ILE:H     | 6        | 0.7           |
| (1,605)  | 1:A:123:ARG:HD3  | 1:A:98:ILE:H     | 6        | 0.7           |
| (1,598)  | 1:A:122:TYR:HB2  | 1:A:122:TYR:H    | 6        | 0.7           |
| (1,598)  | 1:A:122:TYR:HB3  | 1:A:122:TYR:H    | 6        | 0.7           |
| (1,597)  | 1:A:122:TYR:HB2  | 1:A:122:TYR:H    | 6        | 0.7           |
| (1,597)  | 1:A:122:TYR:HB3  | 1:A:122:TYR:H    | 6        | 0.7           |
| (1,592)  | 1:A:122:TYR:HA   | 1:A:122:TYR:HD1  | 6        | 0.7           |
| (1,592)  | 1:A:122:TYR:HA   | 1:A:122:TYR:HD2  | 6        | 0.7           |
| (1,590)  | 1:A:122:TYR:HA   | 1:A:98:ILE:H     | 1        | 0.7           |
| (1,548)  | 1:A:117:GLU:HA   | 1:A:118:PHE:H    | 4        | 0.7           |
| (1,511)  | 1:A:114:ILE:HG21 | 1:A:112:GLY:H    | 3        | 0.7           |
| (1,511)  | 1:A:114:ILE:HG22 | 1:A:112:GLY:H    | 3        | 0.7           |
| (1,511)  | 1:A:114:ILE:HG23 | 1:A:112:GLY:H    | 3        | 0.7           |
| (1,476)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 6        | 0.7           |
| (1,475)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 6        | 0.7           |
| (1,452)  | 1:A:109:ASP:H    | 1:A:114:ILE:HG13 | 8        | 0.7           |
| (1,451)  | 1:A:109:ASP:H    | 1:A:112:GLY:H    | 2        | 0.7           |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD2   | 5        | 0.7           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD3  | 5        | 0.7           |
| (1,256)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2 | 1        | 0.7           |
| (1,255)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2 | 1        | 0.7           |
| (1,251)  | 1:A:89:LEU:HG    | 1:A:90:LYS:H    | 7        | 0.7           |
| (1,1715) | 1:B:147:GLY:HA3  | 1:B:147:GLY:H   | 8        | 0.7           |
| (1,1686) | 1:B:145:VAL:HG21 | 1:B:145:VAL:H   | 2        | 0.7           |
| (1,1686) | 1:B:145:VAL:HG22 | 1:B:145:VAL:H   | 2        | 0.7           |
| (1,1686) | 1:B:145:VAL:HG23 | 1:B:145:VAL:H   | 2        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD1 | 4        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD2 | 4        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD1 | 4        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD2 | 4        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD1 | 4        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD2 | 4        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD1 | 6        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG11  | 1:A:118:PHE:HD2 | 6        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD1 | 6        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG12  | 1:A:118:PHE:HD2 | 6        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD1 | 6        | 0.7           |
| (1,166)  | 1:A:81:VAL:HG13  | 1:A:118:PHE:HD2 | 6        | 0.7           |
| (1,1499) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA  | 2        | 0.7           |
| (1,1499) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA  | 2        | 0.7           |
| (1,1499) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA  | 2        | 0.7           |
| (1,1499) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA  | 9        | 0.7           |
| (1,1499) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA  | 9        | 0.7           |
| (1,1499) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA  | 9        | 0.7           |
| (1,1498) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA  | 2        | 0.7           |
| (1,1498) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA  | 2        | 0.7           |
| (1,1498) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA  | 2        | 0.7           |
| (1,1498) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA  | 9        | 0.7           |
| (1,1498) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA  | 9        | 0.7           |
| (1,1498) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA  | 9        | 0.7           |
| (1,149)  | 1:A:80:ASP:HA    | 1:A:81:VAL:H    | 1        | 0.7           |
| (1,149)  | 1:A:80:ASP:HA    | 1:A:81:VAL:H    | 2        | 0.7           |
| (1,149)  | 1:A:80:ASP:HA    | 1:A:81:VAL:H    | 4        | 0.7           |
| (1,149)  | 1:A:80:ASP:HA    | 1:A:81:VAL:H    | 5        | 0.7           |
| (1,1465) | 1:B:122:TYR:HB2  | 1:B:122:TYR:H   | 6        | 0.7           |
| (1,1465) | 1:B:122:TYR:HB3  | 1:B:122:TYR:H   | 6        | 0.7           |
| (1,1464) | 1:B:122:TYR:HB2  | 1:B:122:TYR:H   | 6        | 0.7           |
| (1,1464) | 1:B:122:TYR:HB3  | 1:B:122:TYR:H   | 6        | 0.7           |
| (1,1459) | 1:B:122:TYR:HA   | 1:B:122:TYR:HD1 | 6        | 0.7           |
| (1,1459) | 1:B:122:TYR:HA   | 1:B:122:TYR:HD2 | 6        | 0.7           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1457) | 1:B:122:TYR:HA   | 1:B:98:ILE:H     | 1        | 0.7           |
| (1,143)  | 1:A:79:LEU:HG    | 1:A:80:ASP:H     | 2        | 0.7           |
| (1,143)  | 1:A:79:LEU:HG    | 1:A:80:ASP:H     | 4        | 0.7           |
| (1,1415) | 1:B:117:GLU:HA   | 1:B:118:PHE:H    | 4        | 0.7           |
| (1,1378) | 1:B:114:ILE:HG21 | 1:B:112:GLY:H    | 3        | 0.7           |
| (1,1378) | 1:B:114:ILE:HG22 | 1:B:112:GLY:H    | 3        | 0.7           |
| (1,1378) | 1:B:114:ILE:HG23 | 1:B:112:GLY:H    | 3        | 0.7           |
| (1,1343) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 6        | 0.7           |
| (1,1342) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 6        | 0.7           |
| (1,1319) | 1:B:109:ASP:H    | 1:B:114:ILE:HG13 | 8        | 0.7           |
| (1,1318) | 1:B:109:ASP:H    | 1:B:112:GLY:H    | 2        | 0.7           |
| (1,1123) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2  | 1        | 0.7           |
| (1,1122) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2  | 1        | 0.7           |
| (1,1118) | 1:B:89:LEU:HG    | 1:B:90:LYS:H     | 7        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG11  | 1:B:118:PHE:HD1  | 4        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG11  | 1:B:118:PHE:HD2  | 4        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG12  | 1:B:118:PHE:HD1  | 4        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG12  | 1:B:118:PHE:HD2  | 4        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG13  | 1:B:118:PHE:HD1  | 4        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG13  | 1:B:118:PHE:HD2  | 4        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG11  | 1:B:118:PHE:HD1  | 6        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG11  | 1:B:118:PHE:HD2  | 6        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG12  | 1:B:118:PHE:HD1  | 6        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG12  | 1:B:118:PHE:HD2  | 6        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG13  | 1:B:118:PHE:HD1  | 6        | 0.7           |
| (1,1033) | 1:B:81:VAL:HG13  | 1:B:118:PHE:HD2  | 6        | 0.7           |
| (1,1016) | 1:B:80:ASP:HA    | 1:B:81:VAL:H     | 1        | 0.7           |
| (1,1016) | 1:B:80:ASP:HA    | 1:B:81:VAL:H     | 2        | 0.7           |
| (1,1016) | 1:B:80:ASP:HA    | 1:B:81:VAL:H     | 4        | 0.7           |
| (1,1016) | 1:B:80:ASP:HA    | 1:B:81:VAL:H     | 5        | 0.7           |
| (1,1010) | 1:B:79:LEU:HG    | 1:B:80:ASP:H     | 2        | 0.7           |
| (1,1010) | 1:B:79:LEU:HG    | 1:B:80:ASP:H     | 4        | 0.7           |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 3        | 0.69          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 3        | 0.69          |
| (1,962)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 3        | 0.69          |
| (1,956)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 3        | 0.69          |
| (1,956)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 3        | 0.69          |
| (1,956)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 3        | 0.69          |
| (1,908)  | 1:B:74:ARG:HG2   | 1:B:74:ARG:H     | 1        | 0.69          |
| (1,908)  | 1:B:74:ARG:HG3   | 1:B:74:ARG:H     | 1        | 0.69          |
| (1,855)  | 1:A:149:ARG:HB2  | 1:A:149:ARG:H    | 7        | 0.69          |
| (1,855)  | 1:A:149:ARG:HB3  | 1:A:149:ARG:H    | 7        | 0.69          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,848) | 1:A:147:GLY:HA3  | 1:A:147:GLY:H    | 7        | 0.69          |
| (1,754) | 1:A:137:LEU:H    | 1:A:137:LEU:HD11 | 2        | 0.69          |
| (1,754) | 1:A:137:LEU:H    | 1:A:137:LEU:HD12 | 2        | 0.69          |
| (1,754) | 1:A:137:LEU:H    | 1:A:137:LEU:HD13 | 2        | 0.69          |
| (1,754) | 1:A:137:LEU:H    | 1:A:137:LEU:HD21 | 2        | 0.69          |
| (1,754) | 1:A:137:LEU:H    | 1:A:137:LEU:HD22 | 2        | 0.69          |
| (1,754) | 1:A:137:LEU:H    | 1:A:137:LEU:HD23 | 2        | 0.69          |
| (1,744) | 1:A:135:SER:HB3  | 1:A:146:ASP:H    | 5        | 0.69          |
| (1,714) | 1:A:133:ILE:HD11 | 1:A:130:PRO:HA   | 6        | 0.69          |
| (1,714) | 1:A:133:ILE:HD12 | 1:A:130:PRO:HA   | 6        | 0.69          |
| (1,714) | 1:A:133:ILE:HD13 | 1:A:130:PRO:HA   | 6        | 0.69          |
| (1,710) | 1:A:132:THR:HB   | 1:A:148:PRO:HD2  | 1        | 0.69          |
| (1,710) | 1:A:132:THR:HB   | 1:A:148:PRO:HD3  | 1        | 0.69          |
| (1,632) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 8        | 0.69          |
| (1,632) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 8        | 0.69          |
| (1,632) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 8        | 0.69          |
| (1,631) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 8        | 0.69          |
| (1,631) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 8        | 0.69          |
| (1,631) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 8        | 0.69          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB2  | 7        | 0.69          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB3  | 7        | 0.69          |
| (1,583) | 1:A:121:LYS:HA   | 1:A:99:GLU:HA    | 4        | 0.69          |
| (1,565) | 1:A:118:PHE:HB2  | 1:A:119:HIS:H    | 9        | 0.69          |
| (1,564) | 1:A:118:PHE:HD1  | 1:A:118:PHE:H    | 1        | 0.69          |
| (1,564) | 1:A:118:PHE:HD2  | 1:A:118:PHE:H    | 1        | 0.69          |
| (1,550) | 1:A:118:PHE:HE1  | 1:A:102:GLY:H    | 2        | 0.69          |
| (1,550) | 1:A:118:PHE:HE2  | 1:A:102:GLY:H    | 2        | 0.69          |
| (1,548) | 1:A:117:GLU:HA   | 1:A:118:PHE:H    | 1        | 0.69          |
| (1,548) | 1:A:117:GLU:HA   | 1:A:118:PHE:H    | 5        | 0.69          |
| (1,547) | 1:A:117:GLU:H    | 1:A:117:GLU:HG2  | 3        | 0.69          |
| (1,547) | 1:A:117:GLU:H    | 1:A:117:GLU:HG3  | 3        | 0.69          |
| (1,476) | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 1        | 0.69          |
| (1,476) | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 4        | 0.69          |
| (1,476) | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 5        | 0.69          |
| (1,475) | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 1        | 0.69          |
| (1,475) | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 4        | 0.69          |
| (1,475) | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 5        | 0.69          |
| (1,41)  | 1:A:74:ARG:HG2   | 1:A:74:ARG:H     | 1        | 0.69          |
| (1,41)  | 1:A:74:ARG:HG3   | 1:A:74:ARG:H     | 1        | 0.69          |
| (1,394) | 1:A:103:LYS:HA   | 1:A:103:LYS:HD2  | 5        | 0.69          |
| (1,394) | 1:A:103:LYS:HA   | 1:A:103:LYS:HD3  | 5        | 0.69          |
| (1,394) | 1:A:103:LYS:HA   | 1:A:103:LYS:HD2  | 9        | 0.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD3  | 9        | 0.69          |
| (1,381)  | 1:A:101:HIS:HA   | 1:A:102:GLY:H    | 6        | 0.69          |
| (1,355)  | 1:A:99:GLU:HB2   | 1:A:121:LYS:HG2  | 2        | 0.69          |
| (1,355)  | 1:A:99:GLU:HB2   | 1:A:121:LYS:HG3  | 2        | 0.69          |
| (1,355)  | 1:A:99:GLU:HB3   | 1:A:121:LYS:HG2  | 2        | 0.69          |
| (1,355)  | 1:A:99:GLU:HB3   | 1:A:121:LYS:HG3  | 2        | 0.69          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG21  | 9        | 0.69          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG22  | 9        | 0.69          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG23  | 9        | 0.69          |
| (1,1722) | 1:B:149:ARG:HB2  | 1:B:149:ARG:H    | 7        | 0.69          |
| (1,1722) | 1:B:149:ARG:HB3  | 1:B:149:ARG:H    | 7        | 0.69          |
| (1,1715) | 1:B:147:GLY:HA3  | 1:B:147:GLY:H    | 7        | 0.69          |
| (1,1621) | 1:B:137:LEU:H    | 1:B:137:LEU:HD11 | 2        | 0.69          |
| (1,1621) | 1:B:137:LEU:H    | 1:B:137:LEU:HD12 | 2        | 0.69          |
| (1,1621) | 1:B:137:LEU:H    | 1:B:137:LEU:HD13 | 2        | 0.69          |
| (1,1621) | 1:B:137:LEU:H    | 1:B:137:LEU:HD21 | 2        | 0.69          |
| (1,1621) | 1:B:137:LEU:H    | 1:B:137:LEU:HD22 | 2        | 0.69          |
| (1,1621) | 1:B:137:LEU:H    | 1:B:137:LEU:HD23 | 2        | 0.69          |
| (1,1611) | 1:B:135:SER:HB3  | 1:B:146:ASP:H    | 5        | 0.69          |
| (1,160)  | 1:A:81:VAL:H     | 1:A:82:LYS:H     | 5        | 0.69          |
| (1,159)  | 1:A:81:VAL:H     | 1:A:82:LYS:H     | 5        | 0.69          |
| (1,1581) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HA   | 6        | 0.69          |
| (1,1581) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HA   | 6        | 0.69          |
| (1,1581) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HA   | 6        | 0.69          |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD2  | 1        | 0.69          |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD3  | 1        | 0.69          |
| (1,157)  | 1:A:81:VAL:HG21  | 1:A:81:VAL:H     | 8        | 0.69          |
| (1,157)  | 1:A:81:VAL:HG22  | 1:A:81:VAL:H     | 8        | 0.69          |
| (1,157)  | 1:A:81:VAL:HG23  | 1:A:81:VAL:H     | 8        | 0.69          |
| (1,1499) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 8        | 0.69          |
| (1,1499) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 8        | 0.69          |
| (1,1499) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 8        | 0.69          |
| (1,1498) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 8        | 0.69          |
| (1,1498) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 8        | 0.69          |
| (1,1498) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 8        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD11 | 4        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD12 | 4        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD13 | 4        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD11 | 4        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD12 | 4        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD13 | 4        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD11 | 4        | 0.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD12 | 4        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD13 | 4        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD11 | 6        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD12 | 6        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD13 | 6        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD11 | 6        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD12 | 6        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD13 | 6        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD11 | 6        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD12 | 6        | 0.69          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD13 | 6        | 0.69          |
| (1,149)  | 1:A:80:ASP:HA    | 1:A:81:VAL:H     | 6        | 0.69          |
| (1,1450) | 1:B:121:LYS:HA   | 1:B:99:GLU:HA    | 4        | 0.69          |
| (1,1432) | 1:B:118:PHE:HB2  | 1:B:119:HIS:H    | 9        | 0.69          |
| (1,1431) | 1:B:118:PHE:HD1  | 1:B:118:PHE:H    | 1        | 0.69          |
| (1,1431) | 1:B:118:PHE:HD2  | 1:B:118:PHE:H    | 1        | 0.69          |
| (1,1425) | 1:B:118:PHE:HA   | 1:B:118:PHE:HZ   | 7        | 0.69          |
| (1,1417) | 1:B:118:PHE:HE1  | 1:B:102:GLY:H    | 2        | 0.69          |
| (1,1417) | 1:B:118:PHE:HE2  | 1:B:102:GLY:H    | 2        | 0.69          |
| (1,1415) | 1:B:117:GLU:HA   | 1:B:118:PHE:H    | 1        | 0.69          |
| (1,1415) | 1:B:117:GLU:HA   | 1:B:118:PHE:H    | 5        | 0.69          |
| (1,1343) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 1        | 0.69          |
| (1,1343) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 4        | 0.69          |
| (1,1343) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 5        | 0.69          |
| (1,1342) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 1        | 0.69          |
| (1,1342) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 4        | 0.69          |
| (1,1342) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 5        | 0.69          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD2  | 5        | 0.69          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD3  | 5        | 0.69          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD2  | 8        | 0.69          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD3  | 8        | 0.69          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD2  | 9        | 0.69          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD3  | 9        | 0.69          |
| (1,1248) | 1:B:101:HIS:HA   | 1:B:102:GLY:H    | 6        | 0.69          |
| (1,1222) | 1:B:99:GLU:HB2   | 1:B:121:LYS:HG2  | 2        | 0.69          |
| (1,1222) | 1:B:99:GLU:HB2   | 1:B:121:LYS:HG3  | 2        | 0.69          |
| (1,1222) | 1:B:99:GLU:HB3   | 1:B:121:LYS:HG2  | 2        | 0.69          |
| (1,1222) | 1:B:99:GLU:HB3   | 1:B:121:LYS:HG3  | 2        | 0.69          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG21  | 9        | 0.69          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG22  | 9        | 0.69          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG23  | 9        | 0.69          |
| (1,1027) | 1:B:81:VAL:H     | 1:B:82:LYS:H     | 5        | 0.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1026) | 1:B:81:VAL:H     | 1:B:82:LYS:H     | 5        | 0.69          |
| (1,1024) | 1:B:81:VAL:HG21  | 1:B:81:VAL:H     | 8        | 0.69          |
| (1,1024) | 1:B:81:VAL:HG22  | 1:B:81:VAL:H     | 8        | 0.69          |
| (1,1024) | 1:B:81:VAL:HG23  | 1:B:81:VAL:H     | 8        | 0.69          |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG11  | 8        | 0.68          |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG12  | 8        | 0.68          |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG13  | 8        | 0.68          |
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG11  | 8        | 0.68          |
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG12  | 8        | 0.68          |
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG13  | 8        | 0.68          |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG11  | 8        | 0.68          |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG12  | 8        | 0.68          |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG13  | 8        | 0.68          |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG11  | 8        | 0.68          |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG12  | 8        | 0.68          |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG13  | 8        | 0.68          |
| (1,831)  | 1:A:146:ASP:HB2  | 1:A:145:VAL:HA   | 4        | 0.68          |
| (1,819)  | 1:A:145:VAL:HG21 | 1:A:145:VAL:H    | 5        | 0.68          |
| (1,819)  | 1:A:145:VAL:HG22 | 1:A:145:VAL:H    | 5        | 0.68          |
| (1,819)  | 1:A:145:VAL:HG23 | 1:A:145:VAL:H    | 5        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD11 | 4        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD12 | 4        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD13 | 4        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD11 | 4        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD12 | 4        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD13 | 4        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD11 | 4        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD12 | 4        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD13 | 4        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD11 | 6        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD12 | 6        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD13 | 6        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD11 | 6        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD12 | 6        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD13 | 6        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD11 | 6        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD12 | 6        | 0.68          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD13 | 6        | 0.68          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD11 | 7        | 0.68          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD12 | 7        | 0.68          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD13 | 7        | 0.68          |
| (1,548)  | 1:A:117:GLU:HA   | 1:A:118:PHE:H    | 2        | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,548)  | 1:A:117:GLU:HA   | 1:A:118:PHE:H    | 6        | 0.68          |
| (1,512)  | 1:A:114:ILE:HD11 | 1:A:113:PHE:HA   | 4        | 0.68          |
| (1,512)  | 1:A:114:ILE:HD12 | 1:A:113:PHE:HA   | 4        | 0.68          |
| (1,512)  | 1:A:114:ILE:HD13 | 1:A:113:PHE:HA   | 4        | 0.68          |
| (1,476)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 3        | 0.68          |
| (1,476)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 8        | 0.68          |
| (1,475)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 3        | 0.68          |
| (1,475)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 8        | 0.68          |
| (1,426)  | 1:A:107:ARG:HD2  | 1:A:107:ARG:H    | 9        | 0.68          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD2  | 4        | 0.68          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD3  | 4        | 0.68          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD2  | 7        | 0.68          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD3  | 7        | 0.68          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD2  | 8        | 0.68          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD3  | 8        | 0.68          |
| (1,355)  | 1:A:99:GLU:HB2   | 1:A:121:LYS:HG2  | 1        | 0.68          |
| (1,355)  | 1:A:99:GLU:HB2   | 1:A:121:LYS:HG3  | 1        | 0.68          |
| (1,355)  | 1:A:99:GLU:HB3   | 1:A:121:LYS:HG2  | 1        | 0.68          |
| (1,355)  | 1:A:99:GLU:HB3   | 1:A:121:LYS:HG3  | 1        | 0.68          |
| (1,355)  | 1:A:99:GLU:HB2   | 1:A:121:LYS:HG2  | 6        | 0.68          |
| (1,355)  | 1:A:99:GLU:HB2   | 1:A:121:LYS:HG3  | 6        | 0.68          |
| (1,355)  | 1:A:99:GLU:HB3   | 1:A:121:LYS:HG2  | 6        | 0.68          |
| (1,355)  | 1:A:99:GLU:HB3   | 1:A:121:LYS:HG3  | 6        | 0.68          |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG21 | 6        | 0.68          |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG22 | 6        | 0.68          |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG23 | 6        | 0.68          |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG21 | 6        | 0.68          |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG22 | 6        | 0.68          |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG23 | 6        | 0.68          |
| (1,288)  | 1:A:93:VAL:HA    | 1:A:99:GLU:H     | 9        | 0.68          |
| (1,239)  | 1:A:89:LEU:H     | 1:A:87:GLU:HA    | 2        | 0.68          |
| (1,212)  | 1:A:85:SER:HB2   | 1:A:88:GLU:H     | 9        | 0.68          |
| (1,1740) | 1:A:113:PHE:HD1  | 1:B:121:LYS:H    | 1        | 0.68          |
| (1,1740) | 1:A:113:PHE:HD2  | 1:B:121:LYS:H    | 1        | 0.68          |
| (1,1698) | 1:B:146:ASP:HB2  | 1:B:145:VAL:HA   | 4        | 0.68          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG21 | 2        | 0.68          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG22 | 2        | 0.68          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG23 | 2        | 0.68          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG21 | 2        | 0.68          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG22 | 2        | 0.68          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG23 | 2        | 0.68          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD11 | 8        | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD12 | 8        | 0.68          |
| (1,1492) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HD13 | 8        | 0.68          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD11 | 8        | 0.68          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD12 | 8        | 0.68          |
| (1,1492) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HD13 | 8        | 0.68          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD11 | 8        | 0.68          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD12 | 8        | 0.68          |
| (1,1492) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HD13 | 8        | 0.68          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD11 | 3        | 0.68          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD12 | 3        | 0.68          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD13 | 3        | 0.68          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD11 | 7        | 0.68          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD12 | 7        | 0.68          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD13 | 7        | 0.68          |
| (1,149)  | 1:A:80:ASP:HA    | 1:A:81:VAL:H     | 3        | 0.68          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB2  | 7        | 0.68          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB3  | 7        | 0.68          |
| (1,1415) | 1:B:117:GLU:HA   | 1:B:118:PHE:H    | 2        | 0.68          |
| (1,1415) | 1:B:117:GLU:HA   | 1:B:118:PHE:H    | 6        | 0.68          |
| (1,1414) | 1:B:117:GLU:H    | 1:B:117:GLU:HG2  | 3        | 0.68          |
| (1,1414) | 1:B:117:GLU:H    | 1:B:117:GLU:HG3  | 3        | 0.68          |
| (1,1379) | 1:B:114:ILE:HD11 | 1:B:113:PHE:HA   | 4        | 0.68          |
| (1,1379) | 1:B:114:ILE:HD12 | 1:B:113:PHE:HA   | 4        | 0.68          |
| (1,1379) | 1:B:114:ILE:HD13 | 1:B:113:PHE:HA   | 4        | 0.68          |
| (1,1343) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 3        | 0.68          |
| (1,1343) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 8        | 0.68          |
| (1,1342) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 3        | 0.68          |
| (1,1342) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 8        | 0.68          |
| (1,1293) | 1:B:107:ARG:HD2  | 1:B:107:ARG:H    | 9        | 0.68          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD2  | 4        | 0.68          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD3  | 4        | 0.68          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD2  | 7        | 0.68          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD3  | 7        | 0.68          |
| (1,1222) | 1:B:99:GLU:HB2   | 1:B:121:LYS:HG2  | 1        | 0.68          |
| (1,1222) | 1:B:99:GLU:HB2   | 1:B:121:LYS:HG3  | 1        | 0.68          |
| (1,1222) | 1:B:99:GLU:HB3   | 1:B:121:LYS:HG2  | 1        | 0.68          |
| (1,1222) | 1:B:99:GLU:HB3   | 1:B:121:LYS:HG3  | 1        | 0.68          |
| (1,1222) | 1:B:99:GLU:HB2   | 1:B:121:LYS:HG2  | 6        | 0.68          |
| (1,1222) | 1:B:99:GLU:HB2   | 1:B:121:LYS:HG3  | 6        | 0.68          |
| (1,1222) | 1:B:99:GLU:HB3   | 1:B:121:LYS:HG2  | 6        | 0.68          |
| (1,1222) | 1:B:99:GLU:HB3   | 1:B:121:LYS:HG3  | 6        | 0.68          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG21 | 6        | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG22 | 6        | 0.68          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG23 | 6        | 0.68          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG21 | 6        | 0.68          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG22 | 6        | 0.68          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG23 | 6        | 0.68          |
| (1,1155) | 1:B:93:VAL:HA    | 1:B:99:GLU:H     | 9        | 0.68          |
| (1,1106) | 1:B:89:LEU:H     | 1:B:87:GLU:HA    | 2        | 0.68          |
| (1,1079) | 1:B:85:SER:HB2   | 1:B:88:GLU:H     | 9        | 0.68          |
| (1,1040) | 1:B:83:HIS:HA    | 1:B:83:HIS:HD2   | 6        | 0.68          |
| (1,1016) | 1:B:80:ASP:HA    | 1:B:81:VAL:H     | 3        | 0.68          |
| (1,1016) | 1:B:80:ASP:HA    | 1:B:81:VAL:H     | 6        | 0.68          |
| (1,1010) | 1:B:79:LEU:HG    | 1:B:80:ASP:H     | 3        | 0.68          |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG11  | 5        | 0.67          |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG12  | 5        | 0.67          |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG13  | 5        | 0.67          |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG11  | 5        | 0.67          |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG12  | 5        | 0.67          |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG13  | 5        | 0.67          |
| (1,758)  | 1:A:138:SER:HA   | 1:A:141:GLY:H    | 2        | 0.67          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG21 | 2        | 0.67          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG22 | 2        | 0.67          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG23 | 2        | 0.67          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG21 | 2        | 0.67          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG22 | 2        | 0.67          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG23 | 2        | 0.67          |
| (1,714)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HA   | 5        | 0.67          |
| (1,714)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HA   | 5        | 0.67          |
| (1,714)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HA   | 5        | 0.67          |
| (1,713)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HB2  | 2        | 0.67          |
| (1,713)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HB3  | 2        | 0.67          |
| (1,713)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HB2  | 2        | 0.67          |
| (1,713)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HB3  | 2        | 0.67          |
| (1,713)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HB2  | 2        | 0.67          |
| (1,713)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HB3  | 2        | 0.67          |
| (1,632)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 3        | 0.67          |
| (1,632)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 3        | 0.67          |
| (1,632)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 3        | 0.67          |
| (1,632)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 7        | 0.67          |
| (1,632)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 7        | 0.67          |
| (1,632)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 7        | 0.67          |
| (1,631)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 3        | 0.67          |
| (1,631)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 3        | 0.67          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,631)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 3        | 0.67          |
| (1,631)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HA   | 7        | 0.67          |
| (1,631)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HA   | 7        | 0.67          |
| (1,631)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HA   | 7        | 0.67          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD11 | 8        | 0.67          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD12 | 8        | 0.67          |
| (1,625)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HD13 | 8        | 0.67          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD11 | 8        | 0.67          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD12 | 8        | 0.67          |
| (1,625)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HD13 | 8        | 0.67          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD11 | 8        | 0.67          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD12 | 8        | 0.67          |
| (1,625)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HD13 | 8        | 0.67          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD11 | 3        | 0.67          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD12 | 3        | 0.67          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD13 | 3        | 0.67          |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB2  | 6        | 0.67          |
| (1,522)  | 1:A:115:SER:HB3  | 1:A:105:GLU:HB3  | 6        | 0.67          |
| (1,480)  | 1:A:112:GLY:HA3  | 1:A:113:PHE:H    | 3        | 0.67          |
| (1,476)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 2        | 0.67          |
| (1,476)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 9        | 0.67          |
| (1,475)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 2        | 0.67          |
| (1,475)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 9        | 0.67          |
| (1,426)  | 1:A:107:ARG:HD2  | 1:A:107:ARG:H    | 2        | 0.67          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD2  | 6        | 0.67          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD3  | 6        | 0.67          |
| (1,256)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2  | 6        | 0.67          |
| (1,255)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2  | 6        | 0.67          |
| (1,191)  | 1:A:84:PHE:HD1   | 1:A:82:LYS:H     | 5        | 0.67          |
| (1,191)  | 1:A:84:PHE:HD2   | 1:A:82:LYS:H     | 5        | 0.67          |
| (1,181)  | 1:A:83:HIS:HB2   | 1:A:84:PHE:HB2   | 8        | 0.67          |
| (1,181)  | 1:A:83:HIS:HB2   | 1:A:84:PHE:HB3   | 8        | 0.67          |
| (1,173)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HD2   | 6        | 0.67          |
| (1,1686) | 1:B:145:VAL:HG21 | 1:B:145:VAL:H    | 5        | 0.67          |
| (1,1686) | 1:B:145:VAL:HG22 | 1:B:145:VAL:H    | 5        | 0.67          |
| (1,1686) | 1:B:145:VAL:HG23 | 1:B:145:VAL:H    | 5        | 0.67          |
| (1,1625) | 1:B:138:SER:HA   | 1:B:141:GLY:H    | 2        | 0.67          |
| (1,1581) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HA   | 5        | 0.67          |
| (1,1581) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HA   | 5        | 0.67          |
| (1,1581) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HA   | 5        | 0.67          |
| (1,150)  | 1:A:81:VAL:HG11  | 1:A:79:LEU:HB2   | 8        | 0.67          |
| (1,150)  | 1:A:81:VAL:HG11  | 1:A:79:LEU:HB3   | 8        | 0.67          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,150)  | 1:A:81:VAL:HG12  | 1:A:79:LEU:HB2  | 8        | 0.67          |
| (1,150)  | 1:A:81:VAL:HG12  | 1:A:79:LEU:HB3  | 8        | 0.67          |
| (1,150)  | 1:A:81:VAL:HG13  | 1:A:79:LEU:HB2  | 8        | 0.67          |
| (1,150)  | 1:A:81:VAL:HG13  | 1:A:79:LEU:HB3  | 8        | 0.67          |
| (1,1499) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA  | 3        | 0.67          |
| (1,1499) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA  | 3        | 0.67          |
| (1,1499) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA  | 3        | 0.67          |
| (1,1498) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA  | 3        | 0.67          |
| (1,1498) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA  | 3        | 0.67          |
| (1,1498) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA  | 3        | 0.67          |
| (1,143)  | 1:A:79:LEU:HG    | 1:A:80:ASP:H    | 3        | 0.67          |
| (1,1425) | 1:B:118:PHE:HA   | 1:B:118:PHE:HZ  | 8        | 0.67          |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB2 | 6        | 0.67          |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB3 | 6        | 0.67          |
| (1,1347) | 1:B:112:GLY:HA3  | 1:B:113:PHE:H   | 3        | 0.67          |
| (1,1343) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3 | 2        | 0.67          |
| (1,1343) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3 | 9        | 0.67          |
| (1,1342) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3 | 2        | 0.67          |
| (1,1342) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3 | 9        | 0.67          |
| (1,1293) | 1:B:107:ARG:HD2  | 1:B:107:ARG:H   | 2        | 0.67          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD2 | 6        | 0.67          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD3 | 6        | 0.67          |
| (1,1123) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2 | 6        | 0.67          |
| (1,1122) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2 | 6        | 0.67          |
| (1,1058) | 1:B:84:PHE:HD1   | 1:B:82:LYS:H    | 5        | 0.67          |
| (1,1058) | 1:B:84:PHE:HD2   | 1:B:82:LYS:H    | 5        | 0.67          |
| (1,1017) | 1:B:81:VAL:HG11  | 1:B:79:LEU:HB2  | 8        | 0.67          |
| (1,1017) | 1:B:81:VAL:HG11  | 1:B:79:LEU:HB3  | 8        | 0.67          |
| (1,1017) | 1:B:81:VAL:HG12  | 1:B:79:LEU:HB2  | 8        | 0.67          |
| (1,1017) | 1:B:81:VAL:HG12  | 1:B:79:LEU:HB3  | 8        | 0.67          |
| (1,1017) | 1:B:81:VAL:HG13  | 1:B:79:LEU:HB2  | 8        | 0.67          |
| (1,1017) | 1:B:81:VAL:HG13  | 1:B:79:LEU:HB3  | 8        | 0.67          |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG11 | 4        | 0.66          |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG12 | 4        | 0.66          |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG13 | 4        | 0.66          |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG11 | 5        | 0.66          |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG12 | 5        | 0.66          |
| (1,960)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG13 | 5        | 0.66          |
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG11 | 4        | 0.66          |
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG12 | 4        | 0.66          |
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG13 | 4        | 0.66          |
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG11 | 5        | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG12  | 5        | 0.66          |
| (1,959)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HG13  | 5        | 0.66          |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG11  | 4        | 0.66          |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG12  | 4        | 0.66          |
| (1,93)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG13  | 4        | 0.66          |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG11  | 4        | 0.66          |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG12  | 4        | 0.66          |
| (1,92)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HG13  | 4        | 0.66          |
| (1,884)  | 1:B:70:LEU:H     | 1:B:70:LEU:HB3   | 6        | 0.66          |
| (1,855)  | 1:A:149:ARG:HB2  | 1:A:149:ARG:H    | 6        | 0.66          |
| (1,855)  | 1:A:149:ARG:HB3  | 1:A:149:ARG:H    | 6        | 0.66          |
| (1,831)  | 1:A:146:ASP:HB2  | 1:A:145:VAL:HA   | 5        | 0.66          |
| (1,758)  | 1:A:138:SER:HA   | 1:A:141:GLY:H    | 5        | 0.66          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG21 | 8        | 0.66          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG22 | 8        | 0.66          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG23 | 8        | 0.66          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG21 | 8        | 0.66          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG22 | 8        | 0.66          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG23 | 8        | 0.66          |
| (1,714)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HA   | 1        | 0.66          |
| (1,714)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HA   | 1        | 0.66          |
| (1,714)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HA   | 1        | 0.66          |
| (1,558)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HZ   | 7        | 0.66          |
| (1,558)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HZ   | 8        | 0.66          |
| (1,548)  | 1:A:117:GLU:HA   | 1:A:118:PHE:H    | 9        | 0.66          |
| (1,540)  | 1:A:116:ARG:HA   | 1:A:117:GLU:H    | 2        | 0.66          |
| (1,511)  | 1:A:114:ILE:HG21 | 1:A:112:GLY:H    | 2        | 0.66          |
| (1,511)  | 1:A:114:ILE:HG22 | 1:A:112:GLY:H    | 2        | 0.66          |
| (1,511)  | 1:A:114:ILE:HG23 | 1:A:112:GLY:H    | 2        | 0.66          |
| (1,476)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 7        | 0.66          |
| (1,475)  | 1:A:112:GLY:HA2  | 1:A:112:GLY:HA3  | 7        | 0.66          |
| (1,437)  | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD1  | 9        | 0.66          |
| (1,437)  | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD2  | 9        | 0.66          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD2   | 7        | 0.66          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD3   | 7        | 0.66          |
| (1,180)  | 1:A:83:HIS:HB2   | 1:A:83:HIS:H     | 3        | 0.66          |
| (1,180)  | 1:A:83:HIS:HB2   | 1:A:83:HIS:H     | 7        | 0.66          |
| (1,1745) | 1:A:114:ILE:H    | 1:B:121:LYS:H    | 3        | 0.66          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE1  | 8        | 0.66          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE2  | 8        | 0.66          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE1  | 8        | 0.66          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE2  | 8        | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE1  | 8        | 0.66          |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE2  | 8        | 0.66          |
| (1,1722) | 1:B:149:ARG:HB2  | 1:B:149:ARG:H    | 6        | 0.66          |
| (1,1722) | 1:B:149:ARG:HB3  | 1:B:149:ARG:H    | 6        | 0.66          |
| (1,17)   | 1:A:70:LEU:H     | 1:A:70:LEU:HB3   | 6        | 0.66          |
| (1,1698) | 1:B:146:ASP:HB2  | 1:B:145:VAL:HA   | 5        | 0.66          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG21 | 8        | 0.66          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG22 | 8        | 0.66          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG23 | 8        | 0.66          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG21 | 8        | 0.66          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG22 | 8        | 0.66          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG23 | 8        | 0.66          |
| (1,1581) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HA   | 1        | 0.66          |
| (1,1581) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HA   | 1        | 0.66          |
| (1,1581) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HA   | 1        | 0.66          |
| (1,1499) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 7        | 0.66          |
| (1,1499) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 7        | 0.66          |
| (1,1499) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 7        | 0.66          |
| (1,1498) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HA   | 7        | 0.66          |
| (1,1498) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HA   | 7        | 0.66          |
| (1,1498) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HA   | 7        | 0.66          |
| (1,149)  | 1:A:80:ASP:HA    | 1:A:81:VAL:H     | 8        | 0.66          |
| (1,1415) | 1:B:117:GLU:HA   | 1:B:118:PHE:H    | 9        | 0.66          |
| (1,1407) | 1:B:116:ARG:HA   | 1:B:117:GLU:H    | 2        | 0.66          |
| (1,1378) | 1:B:114:ILE:HG21 | 1:B:112:GLY:H    | 2        | 0.66          |
| (1,1378) | 1:B:114:ILE:HG22 | 1:B:112:GLY:H    | 2        | 0.66          |
| (1,1378) | 1:B:114:ILE:HG23 | 1:B:112:GLY:H    | 2        | 0.66          |
| (1,1343) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 7        | 0.66          |
| (1,1342) | 1:B:112:GLY:HA2  | 1:B:112:GLY:HA3  | 7        | 0.66          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD1  | 9        | 0.66          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD2  | 9        | 0.66          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD2   | 7        | 0.66          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD3   | 7        | 0.66          |
| (1,1048) | 1:B:83:HIS:HB2   | 1:B:84:PHE:HB2   | 8        | 0.66          |
| (1,1048) | 1:B:83:HIS:HB2   | 1:B:84:PHE:HB3   | 8        | 0.66          |
| (1,1047) | 1:B:83:HIS:HB2   | 1:B:83:HIS:H     | 3        | 0.66          |
| (1,1047) | 1:B:83:HIS:HB2   | 1:B:83:HIS:H     | 7        | 0.66          |
| (1,1016) | 1:B:80:ASP:HA    | 1:B:81:VAL:H     | 8        | 0.66          |
| (1,978)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HE1  | 5        | 0.65          |
| (1,978)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HE2  | 5        | 0.65          |
| (1,978)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HE1  | 5        | 0.65          |
| (1,978)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HE2  | 5        | 0.65          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,978) | 1:B:77:VAL:HG13  | 1:B:122:TYR:HE1  | 5        | 0.65          |
| (1,978) | 1:B:77:VAL:HG13  | 1:B:122:TYR:HE2  | 5        | 0.65          |
| (1,972) | 1:B:77:VAL:HG21  | 1:B:79:LEU:HG    | 9        | 0.65          |
| (1,972) | 1:B:77:VAL:HG22  | 1:B:79:LEU:HG    | 9        | 0.65          |
| (1,972) | 1:B:77:VAL:HG23  | 1:B:79:LEU:HG    | 9        | 0.65          |
| (1,962) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 4        | 0.65          |
| (1,962) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 4        | 0.65          |
| (1,962) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 4        | 0.65          |
| (1,962) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 8        | 0.65          |
| (1,962) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 8        | 0.65          |
| (1,962) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 8        | 0.65          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 4        | 0.65          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 4        | 0.65          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 4        | 0.65          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG21  | 8        | 0.65          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG22  | 8        | 0.65          |
| (1,956) | 1:B:77:VAL:HA    | 1:B:77:VAL:HG23  | 8        | 0.65          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 4        | 0.65          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 4        | 0.65          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 4        | 0.65          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 8        | 0.65          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 8        | 0.65          |
| (1,95)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 8        | 0.65          |
| (1,923) | 1:B:75:PHE:HD1   | 1:B:148:PRO:HA   | 5        | 0.65          |
| (1,923) | 1:B:75:PHE:HD2   | 1:B:148:PRO:HA   | 5        | 0.65          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 4        | 0.65          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 4        | 0.65          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 4        | 0.65          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21  | 8        | 0.65          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22  | 8        | 0.65          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23  | 8        | 0.65          |
| (1,857) | 1:A:150:LYS:H    | 1:A:150:LYS:HD2  | 6        | 0.65          |
| (1,857) | 1:A:150:LYS:H    | 1:A:150:LYS:HD3  | 6        | 0.65          |
| (1,855) | 1:A:149:ARG:HB2  | 1:A:149:ARG:H    | 1        | 0.65          |
| (1,855) | 1:A:149:ARG:HB3  | 1:A:149:ARG:H    | 1        | 0.65          |
| (1,855) | 1:A:149:ARG:HB2  | 1:A:149:ARG:H    | 3        | 0.65          |
| (1,855) | 1:A:149:ARG:HB3  | 1:A:149:ARG:H    | 3        | 0.65          |
| (1,762) | 1:A:138:SER:HB2  | 1:A:142:VAL:H    | 4        | 0.65          |
| (1,762) | 1:A:138:SER:HB3  | 1:A:142:VAL:H    | 4        | 0.65          |
| (1,720) | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG21 | 4        | 0.65          |
| (1,720) | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG22 | 4        | 0.65          |
| (1,720) | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG23 | 4        | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG21 | 4        | 0.65          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG22 | 4        | 0.65          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG23 | 4        | 0.65          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG21 | 9        | 0.65          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG22 | 9        | 0.65          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG23 | 9        | 0.65          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG21 | 9        | 0.65          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG22 | 9        | 0.65          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG23 | 9        | 0.65          |
| (1,583)  | 1:A:121:LYS:HA   | 1:A:99:GLU:HA    | 3        | 0.65          |
| (1,583)  | 1:A:121:LYS:HA   | 1:A:99:GLU:HA    | 7        | 0.65          |
| (1,583)  | 1:A:121:LYS:HA   | 1:A:99:GLU:HA    | 9        | 0.65          |
| (1,56)   | 1:A:75:PHE:HD1   | 1:A:148:PRO:HA   | 5        | 0.65          |
| (1,56)   | 1:A:75:PHE:HD2   | 1:A:148:PRO:HA   | 5        | 0.65          |
| (1,540)  | 1:A:116:ARG:HA   | 1:A:117:GLU:H    | 4        | 0.65          |
| (1,540)  | 1:A:116:ARG:HA   | 1:A:117:GLU:H    | 8        | 0.65          |
| (1,511)  | 1:A:114:ILE:HG21 | 1:A:112:GLY:H    | 1        | 0.65          |
| (1,511)  | 1:A:114:ILE:HG22 | 1:A:112:GLY:H    | 1        | 0.65          |
| (1,511)  | 1:A:114:ILE:HG23 | 1:A:112:GLY:H    | 1        | 0.65          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB2  | 2        | 0.65          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB3  | 2        | 0.65          |
| (1,437)  | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD1  | 3        | 0.65          |
| (1,437)  | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD2  | 3        | 0.65          |
| (1,381)  | 1:A:101:HIS:HA   | 1:A:102:GLY:H    | 3        | 0.65          |
| (1,381)  | 1:A:101:HIS:HA   | 1:A:102:GLY:H    | 5        | 0.65          |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG21 | 7        | 0.65          |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG22 | 7        | 0.65          |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG23 | 7        | 0.65          |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG21 | 7        | 0.65          |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG22 | 7        | 0.65          |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG23 | 7        | 0.65          |
| (1,346)  | 1:A:98:ILE:H     | 1:A:122:TYR:H    | 8        | 0.65          |
| (1,345)  | 1:A:98:ILE:H     | 1:A:122:TYR:H    | 8        | 0.65          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE1  | 3        | 0.65          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE2  | 3        | 0.65          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE1  | 3        | 0.65          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE2  | 3        | 0.65          |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE1  | 3        | 0.65          |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE2  | 3        | 0.65          |
| (1,1738) | 1:A:111:HIS:HA   | 1:B:122:TYR:HD1  | 6        | 0.65          |
| (1,1738) | 1:A:111:HIS:HA   | 1:B:122:TYR:HD2  | 6        | 0.65          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD2  | 6        | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD3  | 6        | 0.65          |
| (1,1722) | 1:B:149:ARG:HB2  | 1:B:149:ARG:H    | 1        | 0.65          |
| (1,1722) | 1:B:149:ARG:HB3  | 1:B:149:ARG:H    | 1        | 0.65          |
| (1,1722) | 1:B:149:ARG:HB2  | 1:B:149:ARG:H    | 3        | 0.65          |
| (1,1722) | 1:B:149:ARG:HB3  | 1:B:149:ARG:H    | 3        | 0.65          |
| (1,1629) | 1:B:138:SER:HB2  | 1:B:142:VAL:H    | 4        | 0.65          |
| (1,1629) | 1:B:138:SER:HB3  | 1:B:142:VAL:H    | 4        | 0.65          |
| (1,1625) | 1:B:138:SER:HA   | 1:B:141:GLY:H    | 5        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG21 | 4        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG22 | 4        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG23 | 4        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG21 | 4        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG22 | 4        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG23 | 4        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG21 | 9        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG22 | 9        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG23 | 9        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG21 | 9        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG22 | 9        | 0.65          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG23 | 9        | 0.65          |
| (1,1450) | 1:B:121:LYS:HA   | 1:B:99:GLU:HA    | 3        | 0.65          |
| (1,1450) | 1:B:121:LYS:HA   | 1:B:99:GLU:HA    | 7        | 0.65          |
| (1,1450) | 1:B:121:LYS:HA   | 1:B:99:GLU:HA    | 9        | 0.65          |
| (1,143)  | 1:A:79:LEU:HG    | 1:A:80:ASP:H     | 7        | 0.65          |
| (1,1407) | 1:B:116:ARG:HA   | 1:B:117:GLU:H    | 4        | 0.65          |
| (1,1407) | 1:B:116:ARG:HA   | 1:B:117:GLU:H    | 8        | 0.65          |
| (1,1378) | 1:B:114:ILE:HG21 | 1:B:112:GLY:H    | 1        | 0.65          |
| (1,1378) | 1:B:114:ILE:HG22 | 1:B:112:GLY:H    | 1        | 0.65          |
| (1,1378) | 1:B:114:ILE:HG23 | 1:B:112:GLY:H    | 1        | 0.65          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB2  | 2        | 0.65          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB3  | 2        | 0.65          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD1  | 3        | 0.65          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD2  | 3        | 0.65          |
| (1,1248) | 1:B:101:HIS:HA   | 1:B:102:GLY:H    | 3        | 0.65          |
| (1,1248) | 1:B:101:HIS:HA   | 1:B:102:GLY:H    | 5        | 0.65          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG21 | 7        | 0.65          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG22 | 7        | 0.65          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG23 | 7        | 0.65          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG21 | 7        | 0.65          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG22 | 7        | 0.65          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG23 | 7        | 0.65          |
| (1,1213) | 1:B:98:ILE:H     | 1:B:122:TYR:H    | 8        | 0.65          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1212) | 1:B:98:ILE:H    | 1:B:122:TYR:H   | 8        | 0.65          |
| (1,111)  | 1:A:77:VAL:HG11 | 1:A:122:TYR:HE1 | 5        | 0.65          |
| (1,111)  | 1:A:77:VAL:HG11 | 1:A:122:TYR:HE2 | 5        | 0.65          |
| (1,111)  | 1:A:77:VAL:HG12 | 1:A:122:TYR:HE1 | 5        | 0.65          |
| (1,111)  | 1:A:77:VAL:HG12 | 1:A:122:TYR:HE2 | 5        | 0.65          |
| (1,111)  | 1:A:77:VAL:HG13 | 1:A:122:TYR:HE1 | 5        | 0.65          |
| (1,111)  | 1:A:77:VAL:HG13 | 1:A:122:TYR:HE2 | 5        | 0.65          |
| (1,105)  | 1:A:77:VAL:HG21 | 1:A:79:LEU:HG   | 9        | 0.65          |
| (1,105)  | 1:A:77:VAL:HG22 | 1:A:79:LEU:HG   | 9        | 0.65          |
| (1,105)  | 1:A:77:VAL:HG23 | 1:A:79:LEU:HG   | 9        | 0.65          |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG11 | 1        | 0.64          |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG12 | 1        | 0.64          |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG13 | 1        | 0.64          |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG11 | 3        | 0.64          |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG12 | 3        | 0.64          |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG13 | 3        | 0.64          |
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG11 | 1        | 0.64          |
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG12 | 1        | 0.64          |
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG13 | 1        | 0.64          |
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG11 | 3        | 0.64          |
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG12 | 3        | 0.64          |
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG13 | 3        | 0.64          |
| (1,95)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG21 | 3        | 0.64          |
| (1,95)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG22 | 3        | 0.64          |
| (1,95)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG23 | 3        | 0.64          |
| (1,93)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG11 | 1        | 0.64          |
| (1,93)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG12 | 1        | 0.64          |
| (1,93)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG13 | 1        | 0.64          |
| (1,93)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG11 | 3        | 0.64          |
| (1,93)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG12 | 3        | 0.64          |
| (1,93)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG13 | 3        | 0.64          |
| (1,92)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG11 | 1        | 0.64          |
| (1,92)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG12 | 1        | 0.64          |
| (1,92)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG13 | 1        | 0.64          |
| (1,92)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG11 | 3        | 0.64          |
| (1,92)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG12 | 3        | 0.64          |
| (1,92)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG13 | 3        | 0.64          |
| (1,89)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG21 | 3        | 0.64          |
| (1,89)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG22 | 3        | 0.64          |
| (1,89)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG23 | 3        | 0.64          |
| (1,881)  | 1:B:68:MET:HE1  | 1:B:122:TYR:HD1 | 9        | 0.64          |
| (1,881)  | 1:B:68:MET:HE1  | 1:B:122:TYR:HD2 | 9        | 0.64          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,881) | 1:B:68:MET:HE2   | 1:B:122:TYR:HD1  | 9        | 0.64          |
| (1,881) | 1:B:68:MET:HE2   | 1:B:122:TYR:HD2  | 9        | 0.64          |
| (1,881) | 1:B:68:MET:HE3   | 1:B:122:TYR:HD1  | 9        | 0.64          |
| (1,881) | 1:B:68:MET:HE3   | 1:B:122:TYR:HD2  | 9        | 0.64          |
| (1,811) | 1:A:145:VAL:HB   | 1:A:77:VAL:HB    | 5        | 0.64          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG21 | 1        | 0.64          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG22 | 1        | 0.64          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG23 | 1        | 0.64          |
| (1,720) | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG21 | 1        | 0.64          |
| (1,720) | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG22 | 1        | 0.64          |
| (1,720) | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG23 | 1        | 0.64          |
| (1,720) | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG21 | 1        | 0.64          |
| (1,720) | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG22 | 1        | 0.64          |
| (1,720) | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG23 | 1        | 0.64          |
| (1,720) | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG21 | 6        | 0.64          |
| (1,720) | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG22 | 6        | 0.64          |
| (1,720) | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG23 | 6        | 0.64          |
| (1,720) | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG21 | 6        | 0.64          |
| (1,720) | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG22 | 6        | 0.64          |
| (1,720) | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG23 | 6        | 0.64          |
| (1,700) | 1:A:132:THR:HG21 | 1:A:132:THR:H    | 8        | 0.64          |
| (1,700) | 1:A:132:THR:HG22 | 1:A:132:THR:H    | 8        | 0.64          |
| (1,700) | 1:A:132:THR:HG23 | 1:A:132:THR:H    | 8        | 0.64          |
| (1,699) | 1:A:132:THR:HG1  | 1:A:132:THR:H    | 5        | 0.64          |
| (1,496) | 1:A:113:PHE:HB3  | 1:A:113:PHE:H    | 5        | 0.64          |
| (1,437) | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD1  | 6        | 0.64          |
| (1,437) | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD2  | 6        | 0.64          |
| (1,426) | 1:A:107:ARG:HD2  | 1:A:107:ARG:H    | 1        | 0.64          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG21 | 2        | 0.64          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG22 | 2        | 0.64          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG23 | 2        | 0.64          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG21 | 2        | 0.64          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG22 | 2        | 0.64          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG23 | 2        | 0.64          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG21 | 3        | 0.64          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG22 | 3        | 0.64          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG23 | 3        | 0.64          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG21 | 3        | 0.64          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG22 | 3        | 0.64          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG23 | 3        | 0.64          |
| (1,323) | 1:A:97:VAL:HB    | 1:A:94:LEU:HB2   | 1        | 0.64          |
| (1,323) | 1:A:97:VAL:HB    | 1:A:94:LEU:HB3   | 1        | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,309)  | 1:A:96:ASP:H     | 1:A:95:GLY:H     | 8        | 0.64          |
| (1,194)  | 1:A:84:PHE:HD1   | 1:A:83:HIS:H     | 5        | 0.64          |
| (1,194)  | 1:A:84:PHE:HD2   | 1:A:83:HIS:H     | 5        | 0.64          |
| (1,181)  | 1:A:83:HIS:HB2   | 1:A:84:PHE:HB2   | 4        | 0.64          |
| (1,181)  | 1:A:83:HIS:HB2   | 1:A:84:PHE:HB3   | 4        | 0.64          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG12 | 1        | 0.64          |
| (1,1757) | 1:A:119:HIS:H    | 1:B:114:ILE:HG13 | 1        | 0.64          |
| (1,1686) | 1:B:145:VAL:HG21 | 1:B:145:VAL:H    | 1        | 0.64          |
| (1,1686) | 1:B:145:VAL:HG22 | 1:B:145:VAL:H    | 1        | 0.64          |
| (1,1686) | 1:B:145:VAL:HG23 | 1:B:145:VAL:H    | 1        | 0.64          |
| (1,1678) | 1:B:145:VAL:HB   | 1:B:77:VAL:HB    | 5        | 0.64          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG21 | 1        | 0.64          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG22 | 1        | 0.64          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG23 | 1        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG21 | 1        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG22 | 1        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG23 | 1        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG21 | 1        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG22 | 1        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG23 | 1        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG21 | 6        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG22 | 6        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG23 | 6        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG21 | 6        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG22 | 6        | 0.64          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG23 | 6        | 0.64          |
| (1,157)  | 1:A:81:VAL:HG21  | 1:A:81:VAL:H     | 2        | 0.64          |
| (1,157)  | 1:A:81:VAL:HG22  | 1:A:81:VAL:H     | 2        | 0.64          |
| (1,157)  | 1:A:81:VAL:HG23  | 1:A:81:VAL:H     | 2        | 0.64          |
| (1,1567) | 1:B:132:THR:HG21 | 1:B:132:THR:H    | 8        | 0.64          |
| (1,1567) | 1:B:132:THR:HG22 | 1:B:132:THR:H    | 8        | 0.64          |
| (1,1567) | 1:B:132:THR:HG23 | 1:B:132:THR:H    | 8        | 0.64          |
| (1,1527) | 1:B:126:ALA:HA   | 1:B:128:VAL:H    | 8        | 0.64          |
| (1,151)  | 1:A:81:VAL:HG11  | 1:A:79:LEU:HG    | 5        | 0.64          |
| (1,151)  | 1:A:81:VAL:HG12  | 1:A:79:LEU:HG    | 5        | 0.64          |
| (1,151)  | 1:A:81:VAL:HG13  | 1:A:79:LEU:HG    | 5        | 0.64          |
| (1,14)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HD1  | 9        | 0.64          |
| (1,14)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HD2  | 9        | 0.64          |
| (1,14)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HD1  | 9        | 0.64          |
| (1,14)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HD2  | 9        | 0.64          |
| (1,14)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HD1  | 9        | 0.64          |
| (1,14)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HD2  | 9        | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1363) | 1:B:113:PHE:HB3  | 1:B:113:PHE:H    | 5        | 0.64          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD1  | 6        | 0.64          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD2  | 6        | 0.64          |
| (1,1293) | 1:B:107:ARG:HD2  | 1:B:107:ARG:H    | 1        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG21 | 2        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG22 | 2        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG23 | 2        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG21 | 2        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG22 | 2        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG23 | 2        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG21 | 3        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG22 | 3        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG23 | 3        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG21 | 3        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG22 | 3        | 0.64          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG23 | 3        | 0.64          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB2   | 1        | 0.64          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB3   | 1        | 0.64          |
| (1,1176) | 1:B:96:ASP:H     | 1:B:95:GLY:H     | 8        | 0.64          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD2   | 6        | 0.64          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD3   | 6        | 0.64          |
| (1,1061) | 1:B:84:PHE:HD1   | 1:B:83:HIS:H     | 5        | 0.64          |
| (1,1061) | 1:B:84:PHE:HD2   | 1:B:83:HIS:H     | 5        | 0.64          |
| (1,1048) | 1:B:83:HIS:HB2   | 1:B:84:PHE:HB2   | 4        | 0.64          |
| (1,1048) | 1:B:83:HIS:HB2   | 1:B:84:PHE:HB3   | 4        | 0.64          |
| (1,1024) | 1:B:81:VAL:HG21  | 1:B:81:VAL:H     | 2        | 0.64          |
| (1,1024) | 1:B:81:VAL:HG22  | 1:B:81:VAL:H     | 2        | 0.64          |
| (1,1024) | 1:B:81:VAL:HG23  | 1:B:81:VAL:H     | 2        | 0.64          |
| (1,1018) | 1:B:81:VAL:HG11  | 1:B:79:LEU:HG    | 5        | 0.64          |
| (1,1018) | 1:B:81:VAL:HG12  | 1:B:79:LEU:HG    | 5        | 0.64          |
| (1,1018) | 1:B:81:VAL:HG13  | 1:B:79:LEU:HG    | 5        | 0.64          |
| (1,1010) | 1:B:79:LEU:HG    | 1:B:80:ASP:H     | 7        | 0.64          |
| (1,929)  | 1:B:76:SER:HB3   | 1:B:76:SER:H     | 7        | 0.63          |
| (1,870)  | 1:B:66:SER:HB2   | 1:B:66:SER:H     | 5        | 0.63          |
| (1,840)  | 1:A:146:ASP:HA   | 1:A:147:GLY:H    | 6        | 0.63          |
| (1,819)  | 1:A:145:VAL:HG21 | 1:A:145:VAL:H    | 1        | 0.63          |
| (1,819)  | 1:A:145:VAL:HG22 | 1:A:145:VAL:H    | 1        | 0.63          |
| (1,819)  | 1:A:145:VAL:HG23 | 1:A:145:VAL:H    | 1        | 0.63          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG21 | 5        | 0.63          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG22 | 5        | 0.63          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG23 | 5        | 0.63          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG21 | 5        | 0.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG22 | 5        | 0.63          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG23 | 5        | 0.63          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG21 | 7        | 0.63          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG22 | 7        | 0.63          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG23 | 7        | 0.63          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG21 | 7        | 0.63          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG22 | 7        | 0.63          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG23 | 7        | 0.63          |
| (1,660)  | 1:A:126:ALA:HA   | 1:A:128:VAL:H    | 8        | 0.63          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG21 | 2        | 0.63          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG22 | 2        | 0.63          |
| (1,649)  | 1:A:125:PRO:HD2  | 1:A:124:ILE:HG23 | 2        | 0.63          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD11 | 1        | 0.63          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD12 | 1        | 0.63          |
| (1,624)  | 1:A:124:ILE:HB   | 1:A:124:ILE:HD13 | 1        | 0.63          |
| (1,62)   | 1:A:76:SER:HB3   | 1:A:76:SER:H     | 7        | 0.63          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG11  | 8        | 0.63          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG12  | 8        | 0.63          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG13  | 8        | 0.63          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG21  | 8        | 0.63          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG22  | 8        | 0.63          |
| (1,604)  | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG23  | 8        | 0.63          |
| (1,568)  | 1:A:119:HIS:HB3  | 1:A:101:HIS:HA   | 2        | 0.63          |
| (1,551)  | 1:A:118:PHE:HD1  | 1:A:103:LYS:HA   | 2        | 0.63          |
| (1,551)  | 1:A:118:PHE:HD2  | 1:A:103:LYS:HA   | 2        | 0.63          |
| (1,548)  | 1:A:117:GLU:HA   | 1:A:118:PHE:H    | 8        | 0.63          |
| (1,540)  | 1:A:116:ARG:HA   | 1:A:117:GLU:H    | 9        | 0.63          |
| (1,524)  | 1:A:115:SER:HB2  | 1:A:106:GLU:H    | 3        | 0.63          |
| (1,524)  | 1:A:115:SER:HB2  | 1:A:106:GLU:H    | 4        | 0.63          |
| (1,498)  | 1:A:113:PHE:HB2  | 1:A:113:PHE:H    | 4        | 0.63          |
| (1,443)  | 1:A:108:GLN:HA   | 1:A:109:ASP:H    | 5        | 0.63          |
| (1,443)  | 1:A:108:GLN:HA   | 1:A:109:ASP:H    | 8        | 0.63          |
| (1,381)  | 1:A:101:HIS:HA   | 1:A:102:GLY:H    | 8        | 0.63          |
| (1,346)  | 1:A:98:ILE:H     | 1:A:122:TYR:H    | 9        | 0.63          |
| (1,345)  | 1:A:98:ILE:H     | 1:A:122:TYR:H    | 9        | 0.63          |
| (1,308)  | 1:A:96:ASP:H     | 1:A:95:GLY:H     | 8        | 0.63          |
| (1,3)    | 1:A:66:SER:HB2   | 1:A:66:SER:H     | 5        | 0.63          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD2   | 6        | 0.63          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD3   | 6        | 0.63          |
| (1,271)  | 1:A:91:VAL:HB    | 1:A:92:LYS:H     | 1        | 0.63          |
| (1,1762) | 1:A:122:TYR:HB2  | 1:B:111:HIS:H    | 3        | 0.63          |
| (1,1762) | 1:A:122:TYR:HB3  | 1:B:111:HIS:H    | 3        | 0.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1707) | 1:B:146:ASP:HA   | 1:B:147:GLY:H    | 6        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG21 | 5        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG22 | 5        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG23 | 5        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG21 | 5        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG22 | 5        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG23 | 5        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG21 | 7        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG22 | 7        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG23 | 7        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG21 | 7        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG22 | 7        | 0.63          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG23 | 7        | 0.63          |
| (1,155)  | 1:A:81:VAL:HG11  | 1:A:81:VAL:HA    | 5        | 0.63          |
| (1,155)  | 1:A:81:VAL:HG12  | 1:A:81:VAL:HA    | 5        | 0.63          |
| (1,155)  | 1:A:81:VAL:HG13  | 1:A:81:VAL:HA    | 5        | 0.63          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG21 | 2        | 0.63          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG22 | 2        | 0.63          |
| (1,1516) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HG23 | 2        | 0.63          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD11 | 1        | 0.63          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD12 | 1        | 0.63          |
| (1,1491) | 1:B:124:ILE:HB   | 1:B:124:ILE:HD13 | 1        | 0.63          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG11  | 8        | 0.63          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG12  | 8        | 0.63          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG13  | 8        | 0.63          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG21  | 8        | 0.63          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG22  | 8        | 0.63          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG23  | 8        | 0.63          |
| (1,1418) | 1:B:118:PHE:HD1  | 1:B:103:LYS:HA   | 2        | 0.63          |
| (1,1418) | 1:B:118:PHE:HD2  | 1:B:103:LYS:HA   | 2        | 0.63          |
| (1,1415) | 1:B:117:GLU:HA   | 1:B:118:PHE:H    | 8        | 0.63          |
| (1,1407) | 1:B:116:ARG:HA   | 1:B:117:GLU:H    | 9        | 0.63          |
| (1,1391) | 1:B:115:SER:HB2  | 1:B:106:GLU:H    | 4        | 0.63          |
| (1,1365) | 1:B:113:PHE:HB2  | 1:B:113:PHE:H    | 4        | 0.63          |
| (1,1310) | 1:B:108:GLN:HA   | 1:B:109:ASP:H    | 5        | 0.63          |
| (1,1310) | 1:B:108:GLN:HA   | 1:B:109:ASP:H    | 8        | 0.63          |
| (1,1248) | 1:B:101:HIS:HA   | 1:B:102:GLY:H    | 8        | 0.63          |
| (1,1213) | 1:B:98:ILE:H     | 1:B:122:TYR:H    | 9        | 0.63          |
| (1,1212) | 1:B:98:ILE:H     | 1:B:122:TYR:H    | 9        | 0.63          |
| (1,1175) | 1:B:96:ASP:H     | 1:B:95:GLY:H     | 8        | 0.63          |
| (1,1138) | 1:B:91:VAL:HB    | 1:B:92:LYS:H     | 1        | 0.63          |
| (1,1022) | 1:B:81:VAL:HG11  | 1:B:81:VAL:HA    | 5        | 0.63          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1022) | 1:B:81:VAL:HG12 | 1:B:81:VAL:HA    | 5        | 0.63          |
| (1,1022) | 1:B:81:VAL:HG13 | 1:B:81:VAL:HA    | 5        | 0.63          |
| (1,981)  | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG11 | 1        | 0.62          |
| (1,981)  | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG12 | 1        | 0.62          |
| (1,981)  | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG13 | 1        | 0.62          |
| (1,981)  | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG11 | 1        | 0.62          |
| (1,981)  | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG12 | 1        | 0.62          |
| (1,981)  | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG13 | 1        | 0.62          |
| (1,981)  | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG11 | 1        | 0.62          |
| (1,981)  | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG12 | 1        | 0.62          |
| (1,981)  | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG13 | 1        | 0.62          |
| (1,969)  | 1:B:77:VAL:HG11 | 1:B:78:ASN:H     | 1        | 0.62          |
| (1,969)  | 1:B:77:VAL:HG12 | 1:B:78:ASN:H     | 1        | 0.62          |
| (1,969)  | 1:B:77:VAL:HG13 | 1:B:78:ASN:H     | 1        | 0.62          |
| (1,962)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG21  | 2        | 0.62          |
| (1,962)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG22  | 2        | 0.62          |
| (1,962)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG23  | 2        | 0.62          |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG11  | 7        | 0.62          |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG12  | 7        | 0.62          |
| (1,960)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG13  | 7        | 0.62          |
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG11  | 7        | 0.62          |
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG12  | 7        | 0.62          |
| (1,959)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG13  | 7        | 0.62          |
| (1,956)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG21  | 2        | 0.62          |
| (1,956)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG22  | 2        | 0.62          |
| (1,956)  | 1:B:77:VAL:HA   | 1:B:77:VAL:HG23  | 2        | 0.62          |
| (1,953)  | 1:B:77:VAL:HG21 | 1:B:75:PHE:HZ    | 7        | 0.62          |
| (1,953)  | 1:B:77:VAL:HG22 | 1:B:75:PHE:HZ    | 7        | 0.62          |
| (1,953)  | 1:B:77:VAL:HG23 | 1:B:75:PHE:HZ    | 7        | 0.62          |
| (1,95)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG21  | 2        | 0.62          |
| (1,95)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG22  | 2        | 0.62          |
| (1,95)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG23  | 2        | 0.62          |
| (1,93)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG11  | 7        | 0.62          |
| (1,93)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG12  | 7        | 0.62          |
| (1,93)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG13  | 7        | 0.62          |
| (1,92)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG11  | 7        | 0.62          |
| (1,92)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG12  | 7        | 0.62          |
| (1,92)   | 1:A:77:VAL:HA   | 1:A:77:VAL:HG13  | 7        | 0.62          |
| (1,919)  | 1:B:75:PHE:HE1  | 1:B:98:ILE:HD11  | 3        | 0.62          |
| (1,919)  | 1:B:75:PHE:HE1  | 1:B:98:ILE:HD12  | 3        | 0.62          |
| (1,919)  | 1:B:75:PHE:HE1  | 1:B:98:ILE:HD13  | 3        | 0.62          |
| (1,919)  | 1:B:75:PHE:HE2  | 1:B:98:ILE:HD11  | 3        | 0.62          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,919) | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD12 | 3        | 0.62          |
| (1,919) | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD13 | 3        | 0.62          |
| (1,919) | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD11 | 7        | 0.62          |
| (1,919) | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD12 | 7        | 0.62          |
| (1,919) | 1:B:75:PHE:HE1   | 1:B:98:ILE:HD13 | 7        | 0.62          |
| (1,919) | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD11 | 7        | 0.62          |
| (1,919) | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD12 | 7        | 0.62          |
| (1,919) | 1:B:75:PHE:HE2   | 1:B:98:ILE:HD13 | 7        | 0.62          |
| (1,902) | 1:B:73:ASP:H     | 1:B:74:ARG:HB3  | 3        | 0.62          |
| (1,892) | 1:B:71:GLU:H     | 1:B:71:GLU:HG2  | 1        | 0.62          |
| (1,892) | 1:B:71:GLU:H     | 1:B:71:GLU:HG3  | 1        | 0.62          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG21 | 2        | 0.62          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG22 | 2        | 0.62          |
| (1,89)  | 1:A:77:VAL:HA    | 1:A:77:VAL:HG23 | 2        | 0.62          |
| (1,886) | 1:B:70:LEU:HD11  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,886) | 1:B:70:LEU:HD12  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,886) | 1:B:70:LEU:HD13  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,886) | 1:B:70:LEU:HD21  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,886) | 1:B:70:LEU:HD22  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,886) | 1:B:70:LEU:HD23  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,885) | 1:B:70:LEU:HD11  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,885) | 1:B:70:LEU:HD12  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,885) | 1:B:70:LEU:HD13  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,885) | 1:B:70:LEU:HD21  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,885) | 1:B:70:LEU:HD22  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,885) | 1:B:70:LEU:HD23  | 1:B:70:LEU:H    | 6        | 0.62          |
| (1,86)  | 1:A:77:VAL:HG21  | 1:A:75:PHE:HZ   | 7        | 0.62          |
| (1,86)  | 1:A:77:VAL:HG22  | 1:A:75:PHE:HZ   | 7        | 0.62          |
| (1,86)  | 1:A:77:VAL:HG23  | 1:A:75:PHE:HZ   | 7        | 0.62          |
| (1,840) | 1:A:146:ASP:HA   | 1:A:147:GLY:H   | 1        | 0.62          |
| (1,717) | 1:A:133:ILE:HG21 | 1:A:132:THR:H   | 7        | 0.62          |
| (1,717) | 1:A:133:ILE:HG22 | 1:A:132:THR:H   | 7        | 0.62          |
| (1,717) | 1:A:133:ILE:HG23 | 1:A:132:THR:H   | 7        | 0.62          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB2 | 3        | 0.62          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB3 | 3        | 0.62          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB2 | 9        | 0.62          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB3 | 9        | 0.62          |
| (1,566) | 1:A:118:PHE:HA   | 1:A:119:HIS:H   | 6        | 0.62          |
| (1,540) | 1:A:116:ARG:HA   | 1:A:117:GLU:H   | 6        | 0.62          |
| (1,540) | 1:A:116:ARG:HA   | 1:A:117:GLU:H   | 7        | 0.62          |
| (1,524) | 1:A:115:SER:HB2  | 1:A:106:GLU:H   | 8        | 0.62          |
| (1,52)  | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD11 | 3        | 0.62          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD12 | 3        | 0.62          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD13 | 3        | 0.62          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD11 | 3        | 0.62          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD12 | 3        | 0.62          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD13 | 3        | 0.62          |
| (1,35)   | 1:A:73:ASP:H     | 1:A:74:ARG:HB3  | 3        | 0.62          |
| (1,330)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA  | 5        | 0.62          |
| (1,329)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA  | 5        | 0.62          |
| (1,263)  | 1:A:90:LYS:H     | 1:A:90:LYS:HD2  | 9        | 0.62          |
| (1,263)  | 1:A:90:LYS:H     | 1:A:90:LYS:HD3  | 9        | 0.62          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG2  | 1        | 0.62          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG3  | 1        | 0.62          |
| (1,19)   | 1:A:70:LEU:HD11  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,19)   | 1:A:70:LEU:HD12  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,19)   | 1:A:70:LEU:HD13  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,19)   | 1:A:70:LEU:HD21  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,19)   | 1:A:70:LEU:HD22  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,19)   | 1:A:70:LEU:HD23  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,18)   | 1:A:70:LEU:HD11  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,18)   | 1:A:70:LEU:HD12  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,18)   | 1:A:70:LEU:HD13  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,18)   | 1:A:70:LEU:HD21  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,18)   | 1:A:70:LEU:HD22  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,18)   | 1:A:70:LEU:HD23  | 1:A:70:LEU:H    | 6        | 0.62          |
| (1,1707) | 1:B:146:ASP:HA   | 1:B:147:GLY:H   | 1        | 0.62          |
| (1,170)  | 1:A:83:HIS:H     | 1:A:81:VAL:HB   | 4        | 0.62          |
| (1,160)  | 1:A:81:VAL:H     | 1:A:82:LYS:H    | 3        | 0.62          |
| (1,159)  | 1:A:81:VAL:H     | 1:A:82:LYS:H    | 3        | 0.62          |
| (1,1584) | 1:B:133:ILE:HG21 | 1:B:132:THR:H   | 7        | 0.62          |
| (1,1584) | 1:B:133:ILE:HG22 | 1:B:132:THR:H   | 7        | 0.62          |
| (1,1584) | 1:B:133:ILE:HG23 | 1:B:132:THR:H   | 7        | 0.62          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB2 | 3        | 0.62          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB3 | 3        | 0.62          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB2 | 9        | 0.62          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB3 | 9        | 0.62          |
| (1,1435) | 1:B:119:HIS:HB3  | 1:B:101:HIS:HA  | 2        | 0.62          |
| (1,1433) | 1:B:118:PHE:HA   | 1:B:119:HIS:H   | 6        | 0.62          |
| (1,143)  | 1:A:79:LEU:HG    | 1:A:80:ASP:H    | 1        | 0.62          |
| (1,1407) | 1:B:116:ARG:HA   | 1:B:117:GLU:H   | 6        | 0.62          |
| (1,1407) | 1:B:116:ARG:HA   | 1:B:117:GLU:H   | 7        | 0.62          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB2 | 1        | 0.62          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB3 | 1        | 0.62          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1391) | 1:B:115:SER:HB2  | 1:B:106:GLU:H   | 3        | 0.62          |
| (1,1197) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 5        | 0.62          |
| (1,1196) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 5        | 0.62          |
| (1,1130) | 1:B:90:LYS:H     | 1:B:90:LYS:HD2  | 9        | 0.62          |
| (1,1130) | 1:B:90:LYS:H     | 1:B:90:LYS:HD3  | 9        | 0.62          |
| (1,1037) | 1:B:83:HIS:H     | 1:B:81:VAL:HB   | 4        | 0.62          |
| (1,1027) | 1:B:81:VAL:H     | 1:B:82:LYS:H    | 3        | 0.62          |
| (1,1026) | 1:B:81:VAL:H     | 1:B:82:LYS:H    | 3        | 0.62          |
| (1,102)  | 1:A:77:VAL:HG11  | 1:A:78:ASN:H    | 1        | 0.62          |
| (1,102)  | 1:A:77:VAL:HG12  | 1:A:78:ASN:H    | 1        | 0.62          |
| (1,102)  | 1:A:77:VAL:HG13  | 1:A:78:ASN:H    | 1        | 0.62          |
| (1,1010) | 1:B:79:LEU:HG    | 1:B:80:ASP:H    | 1        | 0.62          |
| (1,930)  | 1:B:76:SER:HB2   | 1:B:77:VAL:H    | 6        | 0.61          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG2  | 9        | 0.61          |
| (1,891)  | 1:B:71:GLU:H     | 1:B:69:ARG:HG3  | 9        | 0.61          |
| (1,841)  | 1:A:147:GLY:HA2  | 1:A:132:THR:HA  | 9        | 0.61          |
| (1,840)  | 1:A:146:ASP:HA   | 1:A:147:GLY:H   | 8        | 0.61          |
| (1,840)  | 1:A:146:ASP:HA   | 1:A:147:GLY:H   | 9        | 0.61          |
| (1,831)  | 1:A:146:ASP:HB2  | 1:A:145:VAL:HA  | 7        | 0.61          |
| (1,811)  | 1:A:145:VAL:HB   | 1:A:77:VAL:HB   | 1        | 0.61          |
| (1,811)  | 1:A:145:VAL:HB   | 1:A:77:VAL:HB   | 2        | 0.61          |
| (1,810)  | 1:A:144:THR:HG21 | 1:A:146:ASP:HB2 | 6        | 0.61          |
| (1,810)  | 1:A:144:THR:HG22 | 1:A:146:ASP:HB2 | 6        | 0.61          |
| (1,810)  | 1:A:144:THR:HG23 | 1:A:146:ASP:HB2 | 6        | 0.61          |
| (1,717)  | 1:A:133:ILE:HG21 | 1:A:132:THR:H   | 1        | 0.61          |
| (1,717)  | 1:A:133:ILE:HG22 | 1:A:132:THR:H   | 1        | 0.61          |
| (1,717)  | 1:A:133:ILE:HG23 | 1:A:132:THR:H   | 1        | 0.61          |
| (1,717)  | 1:A:133:ILE:HG21 | 1:A:132:THR:H   | 2        | 0.61          |
| (1,717)  | 1:A:133:ILE:HG22 | 1:A:132:THR:H   | 2        | 0.61          |
| (1,717)  | 1:A:133:ILE:HG23 | 1:A:132:THR:H   | 2        | 0.61          |
| (1,697)  | 1:A:132:THR:HG21 | 1:A:129:ASP:H   | 8        | 0.61          |
| (1,697)  | 1:A:132:THR:HG22 | 1:A:129:ASP:H   | 8        | 0.61          |
| (1,697)  | 1:A:132:THR:HG23 | 1:A:129:ASP:H   | 8        | 0.61          |
| (1,63)   | 1:A:76:SER:HB2   | 1:A:77:VAL:H    | 6        | 0.61          |
| (1,586)  | 1:A:121:LYS:HA   | 1:A:122:TYR:H   | 7        | 0.61          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB2 | 1        | 0.61          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB3 | 1        | 0.61          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB2 | 7        | 0.61          |
| (1,538)  | 1:A:116:ARG:H    | 1:A:116:ARG:HB3 | 7        | 0.61          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD11 | 7        | 0.61          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD12 | 7        | 0.61          |
| (1,52)   | 1:A:75:PHE:HE1   | 1:A:98:ILE:HD13 | 7        | 0.61          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD11 | 7        | 0.61          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD12 | 7        | 0.61          |
| (1,52)   | 1:A:75:PHE:HE2   | 1:A:98:ILE:HD13 | 7        | 0.61          |
| (1,459)  | 1:A:111:HIS:H    | 1:A:110:GLU:H   | 5        | 0.61          |
| (1,458)  | 1:A:111:HIS:H    | 1:A:110:GLU:H   | 5        | 0.61          |
| (1,443)  | 1:A:108:GLN:HA   | 1:A:109:ASP:H   | 6        | 0.61          |
| (1,309)  | 1:A:96:ASP:H     | 1:A:95:GLY:H    | 2        | 0.61          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD2  | 9        | 0.61          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD3  | 9        | 0.61          |
| (1,259)  | 1:A:89:LEU:HD11  | 1:A:103:LYS:H   | 3        | 0.61          |
| (1,259)  | 1:A:89:LEU:HD12  | 1:A:103:LYS:H   | 3        | 0.61          |
| (1,259)  | 1:A:89:LEU:HD13  | 1:A:103:LYS:H   | 3        | 0.61          |
| (1,243)  | 1:A:89:LEU:HD11  | 1:A:88:GLU:H    | 8        | 0.61          |
| (1,243)  | 1:A:89:LEU:HD12  | 1:A:88:GLU:H    | 8        | 0.61          |
| (1,243)  | 1:A:89:LEU:HD13  | 1:A:88:GLU:H    | 8        | 0.61          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG2  | 9        | 0.61          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG3  | 9        | 0.61          |
| (1,212)  | 1:A:85:SER:HB2   | 1:A:88:GLU:H    | 5        | 0.61          |
| (1,198)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H    | 8        | 0.61          |
| (1,198)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H    | 8        | 0.61          |
| (1,196)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H    | 8        | 0.61          |
| (1,196)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H    | 8        | 0.61          |
| (1,184)  | 1:A:83:HIS:H     | 1:A:84:PHE:H    | 1        | 0.61          |
| (1,183)  | 1:A:83:HIS:H     | 1:A:84:PHE:H    | 1        | 0.61          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD1 | 4        | 0.61          |
| (1,1746) | 1:A:114:ILE:HD11 | 1:B:122:TYR:HD2 | 4        | 0.61          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD1 | 4        | 0.61          |
| (1,1746) | 1:A:114:ILE:HD12 | 1:B:122:TYR:HD2 | 4        | 0.61          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD1 | 4        | 0.61          |
| (1,1746) | 1:A:114:ILE:HD13 | 1:B:122:TYR:HD2 | 4        | 0.61          |
| (1,1707) | 1:B:146:ASP:HA   | 1:B:147:GLY:H   | 8        | 0.61          |
| (1,1707) | 1:B:146:ASP:HA   | 1:B:147:GLY:H   | 9        | 0.61          |
| (1,1698) | 1:B:146:ASP:HB2  | 1:B:145:VAL:HA  | 7        | 0.61          |
| (1,1690) | 1:B:145:VAL:HG21 | 1:B:146:ASP:H   | 3        | 0.61          |
| (1,1690) | 1:B:145:VAL:HG22 | 1:B:146:ASP:H   | 3        | 0.61          |
| (1,1690) | 1:B:145:VAL:HG23 | 1:B:146:ASP:H   | 3        | 0.61          |
| (1,1678) | 1:B:145:VAL:HB   | 1:B:77:VAL:HB   | 1        | 0.61          |
| (1,1678) | 1:B:145:VAL:HB   | 1:B:77:VAL:HB   | 2        | 0.61          |
| (1,1677) | 1:B:144:THR:HG21 | 1:B:146:ASP:HB2 | 6        | 0.61          |
| (1,1677) | 1:B:144:THR:HG22 | 1:B:146:ASP:HB2 | 6        | 0.61          |
| (1,1677) | 1:B:144:THR:HG23 | 1:B:146:ASP:HB2 | 6        | 0.61          |
| (1,1584) | 1:B:133:ILE:HG21 | 1:B:132:THR:H   | 1        | 0.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1584) | 1:B:133:ILE:HG22 | 1:B:132:THR:H    | 1        | 0.61          |
| (1,1584) | 1:B:133:ILE:HG23 | 1:B:132:THR:H    | 1        | 0.61          |
| (1,1564) | 1:B:132:THR:HG21 | 1:B:129:ASP:H    | 8        | 0.61          |
| (1,1564) | 1:B:132:THR:HG22 | 1:B:129:ASP:H    | 8        | 0.61          |
| (1,1564) | 1:B:132:THR:HG23 | 1:B:129:ASP:H    | 8        | 0.61          |
| (1,155)  | 1:A:81:VAL:HG11  | 1:A:81:VAL:HA    | 6        | 0.61          |
| (1,155)  | 1:A:81:VAL:HG12  | 1:A:81:VAL:HA    | 6        | 0.61          |
| (1,155)  | 1:A:81:VAL:HG13  | 1:A:81:VAL:HA    | 6        | 0.61          |
| (1,1453) | 1:B:121:LYS:HA   | 1:B:122:TYR:H    | 7        | 0.61          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB2  | 7        | 0.61          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB3  | 7        | 0.61          |
| (1,1391) | 1:B:115:SER:HB2  | 1:B:106:GLU:H    | 8        | 0.61          |
| (1,1326) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 5        | 0.61          |
| (1,1325) | 1:B:111:HIS:H    | 1:B:110:GLU:H    | 5        | 0.61          |
| (1,1310) | 1:B:108:GLN:HA   | 1:B:109:ASP:H    | 6        | 0.61          |
| (1,1176) | 1:B:96:ASP:H     | 1:B:95:GLY:H     | 2        | 0.61          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD2   | 9        | 0.61          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD3   | 9        | 0.61          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG11 | 1        | 0.61          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG12 | 1        | 0.61          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG13 | 1        | 0.61          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG11 | 1        | 0.61          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG12 | 1        | 0.61          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG13 | 1        | 0.61          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG11 | 1        | 0.61          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG12 | 1        | 0.61          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG13 | 1        | 0.61          |
| (1,1126) | 1:B:89:LEU:HD11  | 1:B:103:LYS:H    | 3        | 0.61          |
| (1,1126) | 1:B:89:LEU:HD12  | 1:B:103:LYS:H    | 3        | 0.61          |
| (1,1126) | 1:B:89:LEU:HD13  | 1:B:103:LYS:H    | 3        | 0.61          |
| (1,1110) | 1:B:89:LEU:HD11  | 1:B:88:GLU:H     | 8        | 0.61          |
| (1,1110) | 1:B:89:LEU:HD12  | 1:B:88:GLU:H     | 8        | 0.61          |
| (1,1110) | 1:B:89:LEU:HD13  | 1:B:88:GLU:H     | 8        | 0.61          |
| (1,1079) | 1:B:85:SER:HB2   | 1:B:88:GLU:H     | 5        | 0.61          |
| (1,1065) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H     | 8        | 0.61          |
| (1,1065) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H     | 8        | 0.61          |
| (1,1063) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H     | 8        | 0.61          |
| (1,1063) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H     | 8        | 0.61          |
| (1,1051) | 1:B:83:HIS:H     | 1:B:84:PHE:H     | 1        | 0.61          |
| (1,1050) | 1:B:83:HIS:H     | 1:B:84:PHE:H     | 1        | 0.61          |
| (1,1027) | 1:B:81:VAL:H     | 1:B:82:LYS:H     | 6        | 0.61          |
| (1,1026) | 1:B:81:VAL:H     | 1:B:82:LYS:H     | 6        | 0.61          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1022) | 1:B:81:VAL:HG11  | 1:B:81:VAL:HA   | 6        | 0.61          |
| (1,1022) | 1:B:81:VAL:HG12  | 1:B:81:VAL:HA   | 6        | 0.61          |
| (1,1022) | 1:B:81:VAL:HG13  | 1:B:81:VAL:HA   | 6        | 0.61          |
| (1,884)  | 1:B:70:LEU:H     | 1:B:70:LEU:HB3  | 2        | 0.6           |
| (1,862)  | 1:A:150:LYS:HG2  | 1:A:151:GLN:H   | 2        | 0.6           |
| (1,862)  | 1:A:150:LYS:HG3  | 1:A:151:GLN:H   | 2        | 0.6           |
| (1,829)  | 1:A:146:ASP:H    | 1:A:134:THR:H   | 3        | 0.6           |
| (1,828)  | 1:A:146:ASP:H    | 1:A:134:THR:H   | 3        | 0.6           |
| (1,823)  | 1:A:145:VAL:HG21 | 1:A:146:ASP:H   | 3        | 0.6           |
| (1,823)  | 1:A:145:VAL:HG22 | 1:A:146:ASP:H   | 3        | 0.6           |
| (1,823)  | 1:A:145:VAL:HG23 | 1:A:146:ASP:H   | 3        | 0.6           |
| (1,744)  | 1:A:135:SER:HB3  | 1:A:146:ASP:H   | 3        | 0.6           |
| (1,744)  | 1:A:135:SER:HB3  | 1:A:146:ASP:H   | 6        | 0.6           |
| (1,724)  | 1:A:133:ILE:HD11 | 1:A:134:THR:H   | 3        | 0.6           |
| (1,724)  | 1:A:133:ILE:HD12 | 1:A:134:THR:H   | 3        | 0.6           |
| (1,724)  | 1:A:133:ILE:HD13 | 1:A:134:THR:H   | 3        | 0.6           |
| (1,555)  | 1:A:118:PHE:HB2  | 1:A:117:GLU:H   | 7        | 0.6           |
| (1,451)  | 1:A:109:ASP:H    | 1:A:112:GLY:H   | 8        | 0.6           |
| (1,443)  | 1:A:108:GLN:HA   | 1:A:109:ASP:H   | 7        | 0.6           |
| (1,437)  | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD1 | 1        | 0.6           |
| (1,437)  | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD2 | 1        | 0.6           |
| (1,330)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA  | 6        | 0.6           |
| (1,329)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA  | 6        | 0.6           |
| (1,323)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HB2  | 6        | 0.6           |
| (1,323)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HB3  | 6        | 0.6           |
| (1,309)  | 1:A:96:ASP:H     | 1:A:95:GLY:H    | 5        | 0.6           |
| (1,308)  | 1:A:96:ASP:H     | 1:A:95:GLY:H    | 2        | 0.6           |
| (1,256)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2 | 9        | 0.6           |
| (1,255)  | 1:A:89:LEU:HA    | 1:A:102:GLY:HA2 | 9        | 0.6           |
| (1,251)  | 1:A:89:LEU:HG    | 1:A:90:LYS:H    | 4        | 0.6           |
| (1,243)  | 1:A:89:LEU:HD11  | 1:A:88:GLU:H    | 2        | 0.6           |
| (1,243)  | 1:A:89:LEU:HD12  | 1:A:88:GLU:H    | 2        | 0.6           |
| (1,243)  | 1:A:89:LEU:HD13  | 1:A:88:GLU:H    | 2        | 0.6           |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD21 | 2        | 0.6           |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD22 | 2        | 0.6           |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD23 | 2        | 0.6           |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD21 | 2        | 0.6           |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD22 | 2        | 0.6           |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD23 | 2        | 0.6           |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG2  | 5        | 0.6           |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG3  | 5        | 0.6           |
| (1,1740) | 1:A:113:PHE:HD1  | 1:B:121:LYS:H   | 4        | 0.6           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1740) | 1:A:113:PHE:HD2  | 1:B:121:LYS:H   | 4        | 0.6           |
| (1,1729) | 1:B:150:LYS:HG2  | 1:B:151:GLN:H   | 2        | 0.6           |
| (1,1729) | 1:B:150:LYS:HG3  | 1:B:151:GLN:H   | 2        | 0.6           |
| (1,1708) | 1:B:147:GLY:HA2  | 1:B:132:THR:HA  | 9        | 0.6           |
| (1,17)   | 1:A:70:LEU:H     | 1:A:70:LEU:HB3  | 2        | 0.6           |
| (1,1696) | 1:B:146:ASP:H    | 1:B:134:THR:H   | 3        | 0.6           |
| (1,1695) | 1:B:146:ASP:H    | 1:B:134:THR:H   | 3        | 0.6           |
| (1,1611) | 1:B:135:SER:HB3  | 1:B:146:ASP:H   | 3        | 0.6           |
| (1,1611) | 1:B:135:SER:HB3  | 1:B:146:ASP:H   | 6        | 0.6           |
| (1,160)  | 1:A:81:VAL:H     | 1:A:82:LYS:H    | 6        | 0.6           |
| (1,1591) | 1:B:133:ILE:HD11 | 1:B:134:THR:H   | 3        | 0.6           |
| (1,1591) | 1:B:133:ILE:HD12 | 1:B:134:THR:H   | 3        | 0.6           |
| (1,1591) | 1:B:133:ILE:HD13 | 1:B:134:THR:H   | 3        | 0.6           |
| (1,159)  | 1:A:81:VAL:H     | 1:A:82:LYS:H    | 6        | 0.6           |
| (1,155)  | 1:A:81:VAL:HG11  | 1:A:81:VAL:HA   | 3        | 0.6           |
| (1,155)  | 1:A:81:VAL:HG12  | 1:A:81:VAL:HA   | 3        | 0.6           |
| (1,155)  | 1:A:81:VAL:HG13  | 1:A:81:VAL:HA   | 3        | 0.6           |
| (1,155)  | 1:A:81:VAL:HG11  | 1:A:81:VAL:HA   | 8        | 0.6           |
| (1,155)  | 1:A:81:VAL:HG12  | 1:A:81:VAL:HA   | 8        | 0.6           |
| (1,155)  | 1:A:81:VAL:HG13  | 1:A:81:VAL:HA   | 8        | 0.6           |
| (1,155)  | 1:A:81:VAL:HG11  | 1:A:81:VAL:HA   | 9        | 0.6           |
| (1,155)  | 1:A:81:VAL:HG12  | 1:A:81:VAL:HA   | 9        | 0.6           |
| (1,155)  | 1:A:81:VAL:HG13  | 1:A:81:VAL:HA   | 9        | 0.6           |
| (1,1422) | 1:B:118:PHE:HB2  | 1:B:117:GLU:H   | 7        | 0.6           |
| (1,1318) | 1:B:109:ASP:H    | 1:B:112:GLY:H   | 8        | 0.6           |
| (1,1310) | 1:B:108:GLN:HA   | 1:B:109:ASP:H   | 7        | 0.6           |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD1 | 1        | 0.6           |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD2 | 1        | 0.6           |
| (1,1197) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 6        | 0.6           |
| (1,1196) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 6        | 0.6           |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB2  | 6        | 0.6           |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB3  | 6        | 0.6           |
| (1,1176) | 1:B:96:ASP:H     | 1:B:95:GLY:H    | 5        | 0.6           |
| (1,1175) | 1:B:96:ASP:H     | 1:B:95:GLY:H    | 2        | 0.6           |
| (1,1123) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2 | 9        | 0.6           |
| (1,1122) | 1:B:89:LEU:HA    | 1:B:102:GLY:HA2 | 9        | 0.6           |
| (1,1118) | 1:B:89:LEU:HG    | 1:B:90:LYS:H    | 4        | 0.6           |
| (1,1110) | 1:B:89:LEU:HD11  | 1:B:88:GLU:H    | 2        | 0.6           |
| (1,1110) | 1:B:89:LEU:HD12  | 1:B:88:GLU:H    | 2        | 0.6           |
| (1,1110) | 1:B:89:LEU:HD13  | 1:B:88:GLU:H    | 2        | 0.6           |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD21 | 2        | 0.6           |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD22 | 2        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD23  | 2        | 0.6           |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD21  | 2        | 0.6           |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD22  | 2        | 0.6           |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD23  | 2        | 0.6           |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG2   | 5        | 0.6           |
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG3   | 5        | 0.6           |
| (1,1022) | 1:B:81:VAL:HG11  | 1:B:81:VAL:HA    | 3        | 0.6           |
| (1,1022) | 1:B:81:VAL:HG12  | 1:B:81:VAL:HA    | 3        | 0.6           |
| (1,1022) | 1:B:81:VAL:HG13  | 1:B:81:VAL:HA    | 3        | 0.6           |
| (1,1022) | 1:B:81:VAL:HG11  | 1:B:81:VAL:HA    | 8        | 0.6           |
| (1,1022) | 1:B:81:VAL:HG12  | 1:B:81:VAL:HA    | 8        | 0.6           |
| (1,1022) | 1:B:81:VAL:HG13  | 1:B:81:VAL:HA    | 8        | 0.6           |
| (1,1022) | 1:B:81:VAL:HG11  | 1:B:81:VAL:HA    | 9        | 0.6           |
| (1,1022) | 1:B:81:VAL:HG12  | 1:B:81:VAL:HA    | 9        | 0.6           |
| (1,1022) | 1:B:81:VAL:HG13  | 1:B:81:VAL:HA    | 9        | 0.6           |
| (1,1020) | 1:B:81:VAL:HG11  | 1:B:80:ASP:HA    | 1        | 0.6           |
| (1,1020) | 1:B:81:VAL:HG12  | 1:B:80:ASP:HA    | 1        | 0.6           |
| (1,1020) | 1:B:81:VAL:HG13  | 1:B:80:ASP:HA    | 1        | 0.6           |
| (1,892)  | 1:B:71:GLU:H     | 1:B:71:GLU:HG2   | 6        | 0.59          |
| (1,892)  | 1:B:71:GLU:H     | 1:B:71:GLU:HG3   | 6        | 0.59          |
| (1,855)  | 1:A:149:ARG:HB2  | 1:A:149:ARG:H    | 2        | 0.59          |
| (1,855)  | 1:A:149:ARG:HB3  | 1:A:149:ARG:H    | 2        | 0.59          |
| (1,855)  | 1:A:149:ARG:HB2  | 1:A:149:ARG:H    | 8        | 0.59          |
| (1,855)  | 1:A:149:ARG:HB3  | 1:A:149:ARG:H    | 8        | 0.59          |
| (1,840)  | 1:A:146:ASP:HA   | 1:A:147:GLY:H    | 7        | 0.59          |
| (1,831)  | 1:A:146:ASP:HB2  | 1:A:145:VAL:HA   | 8        | 0.59          |
| (1,796)  | 1:A:144:THR:HA   | 1:A:79:LEU:HD11  | 5        | 0.59          |
| (1,796)  | 1:A:144:THR:HA   | 1:A:79:LEU:HD12  | 5        | 0.59          |
| (1,796)  | 1:A:144:THR:HA   | 1:A:79:LEU:HD13  | 5        | 0.59          |
| (1,796)  | 1:A:144:THR:HA   | 1:A:79:LEU:HD21  | 5        | 0.59          |
| (1,796)  | 1:A:144:THR:HA   | 1:A:79:LEU:HD22  | 5        | 0.59          |
| (1,796)  | 1:A:144:THR:HA   | 1:A:79:LEU:HD23  | 5        | 0.59          |
| (1,758)  | 1:A:138:SER:HA   | 1:A:141:GLY:H    | 3        | 0.59          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG11 | 6        | 0.59          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG12 | 6        | 0.59          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG13 | 6        | 0.59          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG21 | 6        | 0.59          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG22 | 6        | 0.59          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG23 | 6        | 0.59          |
| (1,635)  | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 6        | 0.59          |
| (1,635)  | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 6        | 0.59          |
| (1,635)  | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 6        | 0.59          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,634)  | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 6        | 0.59          |
| (1,634)  | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 6        | 0.59          |
| (1,634)  | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 6        | 0.59          |
| (1,559)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HD1  | 1        | 0.59          |
| (1,559)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HD2  | 1        | 0.59          |
| (1,443)  | 1:A:108:GLN:HA   | 1:A:109:ASP:H    | 2        | 0.59          |
| (1,443)  | 1:A:108:GLN:HA   | 1:A:109:ASP:H    | 9        | 0.59          |
| (1,354)  | 1:A:99:GLU:HA    | 1:A:100:VAL:H    | 8        | 0.59          |
| (1,308)  | 1:A:96:ASP:H     | 1:A:95:GLY:H     | 5        | 0.59          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG2   | 6        | 0.59          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG3   | 6        | 0.59          |
| (1,244)  | 1:A:89:LEU:HD21  | 1:A:88:GLU:H     | 1        | 0.59          |
| (1,244)  | 1:A:89:LEU:HD22  | 1:A:88:GLU:H     | 1        | 0.59          |
| (1,244)  | 1:A:89:LEU:HD23  | 1:A:88:GLU:H     | 1        | 0.59          |
| (1,198)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 3        | 0.59          |
| (1,198)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 3        | 0.59          |
| (1,196)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 3        | 0.59          |
| (1,196)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 3        | 0.59          |
| (1,1768) | 1:A:122:TYR:HA   | 1:B:112:GLY:H    | 9        | 0.59          |
| (1,1750) | 1:A:115:SER:HB2  | 1:B:119:HIS:HE1  | 6        | 0.59          |
| (1,1722) | 1:B:149:ARG:HB2  | 1:B:149:ARG:H    | 2        | 0.59          |
| (1,1722) | 1:B:149:ARG:HB3  | 1:B:149:ARG:H    | 2        | 0.59          |
| (1,1722) | 1:B:149:ARG:HB2  | 1:B:149:ARG:H    | 8        | 0.59          |
| (1,1722) | 1:B:149:ARG:HB3  | 1:B:149:ARG:H    | 8        | 0.59          |
| (1,1707) | 1:B:146:ASP:HA   | 1:B:147:GLY:H    | 7        | 0.59          |
| (1,1698) | 1:B:146:ASP:HB2  | 1:B:145:VAL:HA   | 8        | 0.59          |
| (1,1663) | 1:B:144:THR:HA   | 1:B:79:LEU:HD11  | 5        | 0.59          |
| (1,1663) | 1:B:144:THR:HA   | 1:B:79:LEU:HD12  | 5        | 0.59          |
| (1,1663) | 1:B:144:THR:HA   | 1:B:79:LEU:HD13  | 5        | 0.59          |
| (1,1663) | 1:B:144:THR:HA   | 1:B:79:LEU:HD21  | 5        | 0.59          |
| (1,1663) | 1:B:144:THR:HA   | 1:B:79:LEU:HD22  | 5        | 0.59          |
| (1,1663) | 1:B:144:THR:HA   | 1:B:79:LEU:HD23  | 5        | 0.59          |
| (1,1625) | 1:B:138:SER:HA   | 1:B:141:GLY:H    | 3        | 0.59          |
| (1,1584) | 1:B:133:ILE:HG21 | 1:B:132:THR:H    | 2        | 0.59          |
| (1,1584) | 1:B:133:ILE:HG22 | 1:B:132:THR:H    | 2        | 0.59          |
| (1,1584) | 1:B:133:ILE:HG23 | 1:B:132:THR:H    | 2        | 0.59          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG11 | 6        | 0.59          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG12 | 6        | 0.59          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG13 | 6        | 0.59          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG21 | 6        | 0.59          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG22 | 6        | 0.59          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG23 | 6        | 0.59          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,154)  | 1:A:81:VAL:HG21  | 1:A:81:VAL:HA   | 7        | 0.59          |
| (1,154)  | 1:A:81:VAL:HG22  | 1:A:81:VAL:HA   | 7        | 0.59          |
| (1,154)  | 1:A:81:VAL:HG23  | 1:A:81:VAL:HA   | 7        | 0.59          |
| (1,153)  | 1:A:81:VAL:HG11  | 1:A:80:ASP:HA   | 1        | 0.59          |
| (1,153)  | 1:A:81:VAL:HG12  | 1:A:80:ASP:HA   | 1        | 0.59          |
| (1,153)  | 1:A:81:VAL:HG13  | 1:A:80:ASP:HA   | 1        | 0.59          |
| (1,1502) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H   | 6        | 0.59          |
| (1,1502) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H   | 6        | 0.59          |
| (1,1502) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H   | 6        | 0.59          |
| (1,1501) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H   | 6        | 0.59          |
| (1,1501) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H   | 6        | 0.59          |
| (1,1501) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H   | 6        | 0.59          |
| (1,1426) | 1:B:118:PHE:HA   | 1:B:118:PHE:HD1 | 1        | 0.59          |
| (1,1426) | 1:B:118:PHE:HA   | 1:B:118:PHE:HD2 | 1        | 0.59          |
| (1,1391) | 1:B:115:SER:HB2  | 1:B:106:GLU:H   | 6        | 0.59          |
| (1,1310) | 1:B:108:GLN:HA   | 1:B:109:ASP:H   | 2        | 0.59          |
| (1,1310) | 1:B:108:GLN:HA   | 1:B:109:ASP:H   | 9        | 0.59          |
| (1,1221) | 1:B:99:GLU:HA    | 1:B:100:VAL:H   | 8        | 0.59          |
| (1,1175) | 1:B:96:ASP:H     | 1:B:95:GLY:H    | 5        | 0.59          |
| (1,111)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HE1 | 4        | 0.59          |
| (1,111)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HE2 | 4        | 0.59          |
| (1,111)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HE1 | 4        | 0.59          |
| (1,111)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HE2 | 4        | 0.59          |
| (1,111)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HE1 | 4        | 0.59          |
| (1,111)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HE2 | 4        | 0.59          |
| (1,1065) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H    | 3        | 0.59          |
| (1,1065) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H    | 3        | 0.59          |
| (1,1063) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H    | 3        | 0.59          |
| (1,1063) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H    | 3        | 0.59          |
| (1,1021) | 1:B:81:VAL:HG21  | 1:B:81:VAL:HA   | 7        | 0.59          |
| (1,1021) | 1:B:81:VAL:HG22  | 1:B:81:VAL:HA   | 7        | 0.59          |
| (1,1021) | 1:B:81:VAL:HG23  | 1:B:81:VAL:HA   | 7        | 0.59          |
| (1,978)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HE1 | 4        | 0.58          |
| (1,978)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HE2 | 4        | 0.58          |
| (1,978)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HE1 | 4        | 0.58          |
| (1,978)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HE2 | 4        | 0.58          |
| (1,978)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HE1 | 4        | 0.58          |
| (1,978)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HE2 | 4        | 0.58          |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB2  | 5        | 0.58          |
| (1,971)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HB3  | 5        | 0.58          |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB2  | 5        | 0.58          |
| (1,971)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HB3  | 5        | 0.58          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,971) | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB2   | 5        | 0.58          |
| (1,971) | 1:B:77:VAL:HG23  | 1:B:79:LEU:HB3   | 5        | 0.58          |
| (1,923) | 1:B:75:PHE:HD1   | 1:B:148:PRO:HA   | 1        | 0.58          |
| (1,923) | 1:B:75:PHE:HD2   | 1:B:148:PRO:HA   | 1        | 0.58          |
| (1,9)   | 1:A:68:MET:HE1   | 1:A:68:MET:H     | 8        | 0.58          |
| (1,9)   | 1:A:68:MET:HE2   | 1:A:68:MET:H     | 8        | 0.58          |
| (1,9)   | 1:A:68:MET:HE3   | 1:A:68:MET:H     | 8        | 0.58          |
| (1,899) | 1:B:73:ASP:H     | 1:B:72:LYS:H     | 3        | 0.58          |
| (1,876) | 1:B:68:MET:HE1   | 1:B:68:MET:H     | 8        | 0.58          |
| (1,876) | 1:B:68:MET:HE2   | 1:B:68:MET:H     | 8        | 0.58          |
| (1,876) | 1:B:68:MET:HE3   | 1:B:68:MET:H     | 8        | 0.58          |
| (1,857) | 1:A:150:LYS:H    | 1:A:150:LYS:HD2  | 3        | 0.58          |
| (1,857) | 1:A:150:LYS:H    | 1:A:150:LYS:HD3  | 3        | 0.58          |
| (1,843) | 1:A:147:GLY:HA2  | 1:A:133:ILE:HB   | 2        | 0.58          |
| (1,841) | 1:A:147:GLY:HA2  | 1:A:132:THR:HA   | 5        | 0.58          |
| (1,813) | 1:A:145:VAL:HA   | 1:A:135:SER:H    | 3        | 0.58          |
| (1,717) | 1:A:133:ILE:HG21 | 1:A:132:THR:H    | 5        | 0.58          |
| (1,717) | 1:A:133:ILE:HG22 | 1:A:132:THR:H    | 5        | 0.58          |
| (1,717) | 1:A:133:ILE:HG23 | 1:A:132:THR:H    | 5        | 0.58          |
| (1,714) | 1:A:133:ILE:HD11 | 1:A:130:PRO:HA   | 8        | 0.58          |
| (1,714) | 1:A:133:ILE:HD12 | 1:A:130:PRO:HA   | 8        | 0.58          |
| (1,714) | 1:A:133:ILE:HD13 | 1:A:130:PRO:HA   | 8        | 0.58          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG11 | 5        | 0.58          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG12 | 5        | 0.58          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG13 | 5        | 0.58          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG21 | 5        | 0.58          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG22 | 5        | 0.58          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG23 | 5        | 0.58          |
| (1,586) | 1:A:121:LYS:HA   | 1:A:122:TYR:H    | 1        | 0.58          |
| (1,583) | 1:A:121:LYS:HA   | 1:A:99:GLU:HA    | 6        | 0.58          |
| (1,579) | 1:A:119:HIS:H    | 1:A:120:ARG:H    | 7        | 0.58          |
| (1,566) | 1:A:118:PHE:HA   | 1:A:119:HIS:H    | 1        | 0.58          |
| (1,56)  | 1:A:75:PHE:HD1   | 1:A:148:PRO:HA   | 1        | 0.58          |
| (1,56)  | 1:A:75:PHE:HD2   | 1:A:148:PRO:HA   | 1        | 0.58          |
| (1,550) | 1:A:118:PHE:HE1  | 1:A:102:GLY:H    | 1        | 0.58          |
| (1,550) | 1:A:118:PHE:HE2  | 1:A:102:GLY:H    | 1        | 0.58          |
| (1,524) | 1:A:115:SER:HB2  | 1:A:106:GLU:H    | 6        | 0.58          |
| (1,516) | 1:A:114:ILE:H    | 1:A:114:ILE:HG12 | 1        | 0.58          |
| (1,443) | 1:A:108:GLN:HA   | 1:A:109:ASP:H    | 4        | 0.58          |
| (1,432) | 1:A:107:ARG:HG2  | 1:A:108:GLN:H    | 5        | 0.58          |
| (1,432) | 1:A:107:ARG:HG3  | 1:A:108:GLN:H    | 5        | 0.58          |
| (1,387) | 1:A:102:GLY:HA3  | 1:A:102:GLY:H    | 1        | 0.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,387)  | 1:A:102:GLY:HA3  | 1:A:102:GLY:H    | 3        | 0.58          |
| (1,354)  | 1:A:99:GLU:HA    | 1:A:100:VAL:H    | 9        | 0.58          |
| (1,32)   | 1:A:73:ASP:H     | 1:A:72:LYS:H     | 3        | 0.58          |
| (1,300)  | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB2   | 2        | 0.58          |
| (1,300)  | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB3   | 2        | 0.58          |
| (1,287)  | 1:A:93:VAL:HA    | 1:A:98:ILE:HA    | 5        | 0.58          |
| (1,271)  | 1:A:91:VAL:HB    | 1:A:92:LYS:H     | 3        | 0.58          |
| (1,198)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 6        | 0.58          |
| (1,198)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 6        | 0.58          |
| (1,196)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 6        | 0.58          |
| (1,196)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 6        | 0.58          |
| (1,195)  | 1:A:84:PHE:HD1   | 1:A:84:PHE:H     | 1        | 0.58          |
| (1,195)  | 1:A:84:PHE:HD2   | 1:A:84:PHE:H     | 1        | 0.58          |
| (1,192)  | 1:A:84:PHE:HD1   | 1:A:83:HIS:HB3   | 4        | 0.58          |
| (1,192)  | 1:A:84:PHE:HD2   | 1:A:83:HIS:HB3   | 4        | 0.58          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD2  | 3        | 0.58          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD3  | 3        | 0.58          |
| (1,1710) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HB   | 2        | 0.58          |
| (1,1708) | 1:B:147:GLY:HA2  | 1:B:132:THR:HA   | 5        | 0.58          |
| (1,1680) | 1:B:145:VAL:HA   | 1:B:135:SER:H    | 3        | 0.58          |
| (1,1584) | 1:B:133:ILE:HG21 | 1:B:132:THR:H    | 5        | 0.58          |
| (1,1584) | 1:B:133:ILE:HG22 | 1:B:132:THR:H    | 5        | 0.58          |
| (1,1584) | 1:B:133:ILE:HG23 | 1:B:132:THR:H    | 5        | 0.58          |
| (1,1581) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HA   | 8        | 0.58          |
| (1,1581) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HA   | 8        | 0.58          |
| (1,1581) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HA   | 8        | 0.58          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG11 | 5        | 0.58          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG12 | 5        | 0.58          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG13 | 5        | 0.58          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG21 | 5        | 0.58          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG22 | 5        | 0.58          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG23 | 5        | 0.58          |
| (1,1453) | 1:B:121:LYS:HA   | 1:B:122:TYR:H    | 1        | 0.58          |
| (1,1450) | 1:B:121:LYS:HA   | 1:B:99:GLU:HA    | 6        | 0.58          |
| (1,1446) | 1:B:119:HIS:H    | 1:B:120:ARG:H    | 7        | 0.58          |
| (1,1433) | 1:B:118:PHE:HA   | 1:B:119:HIS:H    | 1        | 0.58          |
| (1,1417) | 1:B:118:PHE:HE1  | 1:B:102:GLY:H    | 1        | 0.58          |
| (1,1417) | 1:B:118:PHE:HE2  | 1:B:102:GLY:H    | 1        | 0.58          |
| (1,1383) | 1:B:114:ILE:H    | 1:B:114:ILE:HG12 | 1        | 0.58          |
| (1,1310) | 1:B:108:GLN:HA   | 1:B:109:ASP:H    | 3        | 0.58          |
| (1,1310) | 1:B:108:GLN:HA   | 1:B:109:ASP:H    | 4        | 0.58          |
| (1,1299) | 1:B:107:ARG:HG2  | 1:B:108:GLN:H    | 5        | 0.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1299) | 1:B:107:ARG:HG3  | 1:B:108:GLN:H    | 5        | 0.58          |
| (1,1254) | 1:B:102:GLY:HA3  | 1:B:102:GLY:H    | 1        | 0.58          |
| (1,1221) | 1:B:99:GLU:HA    | 1:B:100:VAL:H    | 9        | 0.58          |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB2   | 2        | 0.58          |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB3   | 2        | 0.58          |
| (1,1154) | 1:B:93:VAL:HA    | 1:B:98:ILE:HA    | 5        | 0.58          |
| (1,1138) | 1:B:91:VAL:HB    | 1:B:92:LYS:H     | 3        | 0.58          |
| (1,1111) | 1:B:89:LEU:HD21  | 1:B:88:GLU:H     | 1        | 0.58          |
| (1,1111) | 1:B:89:LEU:HD22  | 1:B:88:GLU:H     | 1        | 0.58          |
| (1,1111) | 1:B:89:LEU:HD23  | 1:B:88:GLU:H     | 1        | 0.58          |
| (1,1065) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H     | 6        | 0.58          |
| (1,1065) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H     | 6        | 0.58          |
| (1,1063) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H     | 6        | 0.58          |
| (1,1063) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H     | 6        | 0.58          |
| (1,1062) | 1:B:84:PHE:HD1   | 1:B:84:PHE:H     | 1        | 0.58          |
| (1,1062) | 1:B:84:PHE:HD2   | 1:B:84:PHE:H     | 1        | 0.58          |
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB2   | 5        | 0.58          |
| (1,104)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HB3   | 5        | 0.58          |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB2   | 5        | 0.58          |
| (1,104)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HB3   | 5        | 0.58          |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB2   | 5        | 0.58          |
| (1,104)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HB3   | 5        | 0.58          |
| (1,974)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HG    | 1        | 0.57          |
| (1,974)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HG    | 1        | 0.57          |
| (1,974)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HG    | 1        | 0.57          |
| (1,974)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HG    | 3        | 0.57          |
| (1,974)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HG    | 3        | 0.57          |
| (1,974)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HG    | 3        | 0.57          |
| (1,97)   | 1:A:77:VAL:HG21  | 1:A:77:VAL:H     | 3        | 0.57          |
| (1,97)   | 1:A:77:VAL:HG22  | 1:A:77:VAL:H     | 3        | 0.57          |
| (1,97)   | 1:A:77:VAL:HG23  | 1:A:77:VAL:H     | 3        | 0.57          |
| (1,902)  | 1:B:73:ASP:H     | 1:B:74:ARG:HB3   | 6        | 0.57          |
| (1,845)  | 1:A:147:GLY:HA2  | 1:A:133:ILE:HD11 | 3        | 0.57          |
| (1,845)  | 1:A:147:GLY:HA2  | 1:A:133:ILE:HD12 | 3        | 0.57          |
| (1,845)  | 1:A:147:GLY:HA2  | 1:A:133:ILE:HD13 | 3        | 0.57          |
| (1,840)  | 1:A:146:ASP:HA   | 1:A:147:GLY:H    | 5        | 0.57          |
| (1,799)  | 1:A:144:THR:HG21 | 1:A:144:THR:HA   | 5        | 0.57          |
| (1,799)  | 1:A:144:THR:HG22 | 1:A:144:THR:HA   | 5        | 0.57          |
| (1,799)  | 1:A:144:THR:HG23 | 1:A:144:THR:HA   | 5        | 0.57          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG21 | 3        | 0.57          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG22 | 3        | 0.57          |
| (1,720)  | 1:A:133:ILE:HG12 | 1:A:133:ILE:HG23 | 3        | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG21 | 3        | 0.57          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG22 | 3        | 0.57          |
| (1,720)  | 1:A:133:ILE:HG13 | 1:A:133:ILE:HG23 | 3        | 0.57          |
| (1,621)  | 1:A:124:ILE:HD11 | 1:A:123:ARG:HA   | 9        | 0.57          |
| (1,621)  | 1:A:124:ILE:HD12 | 1:A:123:ARG:HA   | 9        | 0.57          |
| (1,621)  | 1:A:124:ILE:HD13 | 1:A:123:ARG:HA   | 9        | 0.57          |
| (1,584)  | 1:A:121:LYS:HA   | 1:A:120:ARG:HB2  | 4        | 0.57          |
| (1,584)  | 1:A:121:LYS:HA   | 1:A:120:ARG:HB3  | 4        | 0.57          |
| (1,580)  | 1:A:120:ARG:H    | 1:A:100:VAL:H    | 8        | 0.57          |
| (1,565)  | 1:A:118:PHE:HB2  | 1:A:119:HIS:H    | 4        | 0.57          |
| (1,443)  | 1:A:108:GLN:HA   | 1:A:109:ASP:H    | 3        | 0.57          |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG2   | 7        | 0.57          |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG3   | 7        | 0.57          |
| (1,35)   | 1:A:73:ASP:H     | 1:A:74:ARG:HB3   | 6        | 0.57          |
| (1,330)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA   | 8        | 0.57          |
| (1,329)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA   | 8        | 0.57          |
| (1,321)  | 1:A:97:VAL:H     | 1:A:93:VAL:HB    | 1        | 0.57          |
| (1,309)  | 1:A:96:ASP:H     | 1:A:95:GLY:H     | 6        | 0.57          |
| (1,309)  | 1:A:96:ASP:H     | 1:A:95:GLY:H     | 7        | 0.57          |
| (1,271)  | 1:A:91:VAL:HB    | 1:A:92:LYS:H     | 2        | 0.57          |
| (1,244)  | 1:A:89:LEU:HD21  | 1:A:88:GLU:H     | 6        | 0.57          |
| (1,244)  | 1:A:89:LEU:HD22  | 1:A:88:GLU:H     | 6        | 0.57          |
| (1,244)  | 1:A:89:LEU:HD23  | 1:A:88:GLU:H     | 6        | 0.57          |
| (1,231)  | 1:A:87:GLU:HB2   | 1:A:89:LEU:H     | 5        | 0.57          |
| (1,231)  | 1:A:87:GLU:HB3   | 1:A:89:LEU:H     | 5        | 0.57          |
| (1,198)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 7        | 0.57          |
| (1,198)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 7        | 0.57          |
| (1,196)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 7        | 0.57          |
| (1,196)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 7        | 0.57          |
| (1,180)  | 1:A:83:HIS:HB2   | 1:A:83:HIS:H     | 1        | 0.57          |
| (1,180)  | 1:A:83:HIS:HB2   | 1:A:83:HIS:H     | 9        | 0.57          |
| (1,1712) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HD11 | 3        | 0.57          |
| (1,1712) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HD12 | 3        | 0.57          |
| (1,1712) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HD13 | 3        | 0.57          |
| (1,171)  | 1:A:83:HIS:H     | 1:A:82:LYS:HG2   | 2        | 0.57          |
| (1,171)  | 1:A:83:HIS:H     | 1:A:82:LYS:HG3   | 2        | 0.57          |
| (1,1707) | 1:B:146:ASP:HA   | 1:B:147:GLY:H    | 5        | 0.57          |
| (1,1666) | 1:B:144:THR:HG21 | 1:B:144:THR:HA   | 5        | 0.57          |
| (1,1666) | 1:B:144:THR:HG22 | 1:B:144:THR:HA   | 5        | 0.57          |
| (1,1666) | 1:B:144:THR:HG23 | 1:B:144:THR:HA   | 5        | 0.57          |
| (1,1666) | 1:B:144:THR:HG21 | 1:B:144:THR:HA   | 6        | 0.57          |
| (1,1666) | 1:B:144:THR:HG22 | 1:B:144:THR:HA   | 6        | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1666) | 1:B:144:THR:HG23 | 1:B:144:THR:HA   | 6        | 0.57          |
| (1,163)  | 1:A:81:VAL:HG21  | 1:A:83:HIS:H     | 7        | 0.57          |
| (1,163)  | 1:A:81:VAL:HG22  | 1:A:83:HIS:H     | 7        | 0.57          |
| (1,163)  | 1:A:81:VAL:HG23  | 1:A:83:HIS:H     | 7        | 0.57          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG21 | 3        | 0.57          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG22 | 3        | 0.57          |
| (1,1587) | 1:B:133:ILE:HG12 | 1:B:133:ILE:HG23 | 3        | 0.57          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG21 | 3        | 0.57          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG22 | 3        | 0.57          |
| (1,1587) | 1:B:133:ILE:HG13 | 1:B:133:ILE:HG23 | 3        | 0.57          |
| (1,157)  | 1:A:81:VAL:HG21  | 1:A:81:VAL:H     | 6        | 0.57          |
| (1,157)  | 1:A:81:VAL:HG22  | 1:A:81:VAL:H     | 6        | 0.57          |
| (1,157)  | 1:A:81:VAL:HG23  | 1:A:81:VAL:H     | 6        | 0.57          |
| (1,1488) | 1:B:124:ILE:HD11 | 1:B:123:ARG:HA   | 9        | 0.57          |
| (1,1488) | 1:B:124:ILE:HD12 | 1:B:123:ARG:HA   | 9        | 0.57          |
| (1,1488) | 1:B:124:ILE:HD13 | 1:B:123:ARG:HA   | 9        | 0.57          |
| (1,1457) | 1:B:122:TYR:HA   | 1:B:98:ILE:H     | 4        | 0.57          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB2  | 4        | 0.57          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB3  | 4        | 0.57          |
| (1,1432) | 1:B:118:PHE:HB2  | 1:B:119:HIS:H    | 4        | 0.57          |
| (1,1260) | 1:B:103:LYS:H    | 1:B:88:GLU:HG2   | 7        | 0.57          |
| (1,1260) | 1:B:103:LYS:H    | 1:B:88:GLU:HG3   | 7        | 0.57          |
| (1,1254) | 1:B:102:GLY:HA3  | 1:B:102:GLY:H    | 3        | 0.57          |
| (1,1197) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA   | 8        | 0.57          |
| (1,1196) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA   | 8        | 0.57          |
| (1,1188) | 1:B:97:VAL:H     | 1:B:93:VAL:HB    | 1        | 0.57          |
| (1,1176) | 1:B:96:ASP:H     | 1:B:95:GLY:H     | 1        | 0.57          |
| (1,1176) | 1:B:96:ASP:H     | 1:B:95:GLY:H     | 6        | 0.57          |
| (1,1176) | 1:B:96:ASP:H     | 1:B:95:GLY:H     | 7        | 0.57          |
| (1,1138) | 1:B:91:VAL:HB    | 1:B:92:LYS:H     | 2        | 0.57          |
| (1,1111) | 1:B:89:LEU:HD21  | 1:B:88:GLU:H     | 6        | 0.57          |
| (1,1111) | 1:B:89:LEU:HD22  | 1:B:88:GLU:H     | 6        | 0.57          |
| (1,1111) | 1:B:89:LEU:HD23  | 1:B:88:GLU:H     | 6        | 0.57          |
| (1,1098) | 1:B:87:GLU:HB2   | 1:B:89:LEU:H     | 5        | 0.57          |
| (1,1098) | 1:B:87:GLU:HB3   | 1:B:89:LEU:H     | 5        | 0.57          |
| (1,107)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:HG    | 3        | 0.57          |
| (1,107)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:HG    | 3        | 0.57          |
| (1,107)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:HG    | 3        | 0.57          |
| (1,1065) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H     | 7        | 0.57          |
| (1,1065) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H     | 7        | 0.57          |
| (1,1063) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H     | 7        | 0.57          |
| (1,1063) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H     | 7        | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1059) | 1:B:84:PHE:HD1   | 1:B:83:HIS:HB3   | 4        | 0.57          |
| (1,1059) | 1:B:84:PHE:HD2   | 1:B:83:HIS:HB3   | 4        | 0.57          |
| (1,1047) | 1:B:83:HIS:HB2   | 1:B:83:HIS:H     | 1        | 0.57          |
| (1,1047) | 1:B:83:HIS:HB2   | 1:B:83:HIS:H     | 9        | 0.57          |
| (1,1038) | 1:B:83:HIS:H     | 1:B:82:LYS:HG2   | 2        | 0.57          |
| (1,1038) | 1:B:83:HIS:H     | 1:B:82:LYS:HG3   | 2        | 0.57          |
| (1,1030) | 1:B:81:VAL:HG21  | 1:B:83:HIS:H     | 7        | 0.57          |
| (1,1030) | 1:B:81:VAL:HG22  | 1:B:83:HIS:H     | 7        | 0.57          |
| (1,1030) | 1:B:81:VAL:HG23  | 1:B:83:HIS:H     | 7        | 0.57          |
| (1,1024) | 1:B:81:VAL:HG21  | 1:B:81:VAL:H     | 6        | 0.57          |
| (1,1024) | 1:B:81:VAL:HG22  | 1:B:81:VAL:H     | 6        | 0.57          |
| (1,1024) | 1:B:81:VAL:HG23  | 1:B:81:VAL:H     | 6        | 0.57          |
| (1,1018) | 1:B:81:VAL:HG11  | 1:B:79:LEU:HG    | 2        | 0.57          |
| (1,1018) | 1:B:81:VAL:HG12  | 1:B:79:LEU:HG    | 2        | 0.57          |
| (1,1018) | 1:B:81:VAL:HG13  | 1:B:79:LEU:HG    | 2        | 0.57          |
| (1,986)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB3  | 4        | 0.56          |
| (1,977)  | 1:B:77:VAL:HG11  | 1:B:98:ILE:HD11  | 3        | 0.56          |
| (1,977)  | 1:B:77:VAL:HG11  | 1:B:98:ILE:HD12  | 3        | 0.56          |
| (1,977)  | 1:B:77:VAL:HG11  | 1:B:98:ILE:HD13  | 3        | 0.56          |
| (1,977)  | 1:B:77:VAL:HG12  | 1:B:98:ILE:HD11  | 3        | 0.56          |
| (1,977)  | 1:B:77:VAL:HG12  | 1:B:98:ILE:HD12  | 3        | 0.56          |
| (1,977)  | 1:B:77:VAL:HG12  | 1:B:98:ILE:HD13  | 3        | 0.56          |
| (1,977)  | 1:B:77:VAL:HG13  | 1:B:98:ILE:HD11  | 3        | 0.56          |
| (1,977)  | 1:B:77:VAL:HG13  | 1:B:98:ILE:HD12  | 3        | 0.56          |
| (1,977)  | 1:B:77:VAL:HG13  | 1:B:98:ILE:HD13  | 3        | 0.56          |
| (1,848)  | 1:A:147:GLY:HA3  | 1:A:147:GLY:H    | 9        | 0.56          |
| (1,799)  | 1:A:144:THR:HG21 | 1:A:144:THR:HA   | 6        | 0.56          |
| (1,799)  | 1:A:144:THR:HG22 | 1:A:144:THR:HA   | 6        | 0.56          |
| (1,799)  | 1:A:144:THR:HG23 | 1:A:144:THR:HA   | 6        | 0.56          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD11 | 4        | 0.56          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD12 | 4        | 0.56          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD13 | 4        | 0.56          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD21 | 4        | 0.56          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD22 | 4        | 0.56          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD23 | 4        | 0.56          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG11 | 2        | 0.56          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG12 | 2        | 0.56          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG13 | 2        | 0.56          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG21 | 2        | 0.56          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG22 | 2        | 0.56          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG23 | 2        | 0.56          |
| (1,590)  | 1:A:122:TYR:HA   | 1:A:98:ILE:H     | 4        | 0.56          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,497)  | 1:A:113:PHE:HD1 | 1:A:113:PHE:H    | 7        | 0.56          |
| (1,497)  | 1:A:113:PHE:HD2 | 1:A:113:PHE:H    | 7        | 0.56          |
| (1,481)  | 1:A:113:PHE:HA  | 1:A:107:ARG:HB2  | 4        | 0.56          |
| (1,447)  | 1:A:109:ASP:H   | 1:A:109:ASP:HB2  | 6        | 0.56          |
| (1,447)  | 1:A:109:ASP:H   | 1:A:109:ASP:HB3  | 6        | 0.56          |
| (1,443)  | 1:A:108:GLN:HA  | 1:A:109:ASP:H    | 1        | 0.56          |
| (1,432)  | 1:A:107:ARG:HG2 | 1:A:108:GLN:H    | 7        | 0.56          |
| (1,432)  | 1:A:107:ARG:HG3 | 1:A:108:GLN:H    | 7        | 0.56          |
| (1,387)  | 1:A:102:GLY:HA3 | 1:A:102:GLY:H    | 5        | 0.56          |
| (1,387)  | 1:A:102:GLY:HA3 | 1:A:102:GLY:H    | 6        | 0.56          |
| (1,355)  | 1:A:99:GLU:HB2  | 1:A:121:LYS:HG2  | 5        | 0.56          |
| (1,355)  | 1:A:99:GLU:HB2  | 1:A:121:LYS:HG3  | 5        | 0.56          |
| (1,355)  | 1:A:99:GLU:HB3  | 1:A:121:LYS:HG2  | 5        | 0.56          |
| (1,355)  | 1:A:99:GLU:HB3  | 1:A:121:LYS:HG3  | 5        | 0.56          |
| (1,309)  | 1:A:96:ASP:H    | 1:A:95:GLY:H     | 1        | 0.56          |
| (1,309)  | 1:A:96:ASP:H    | 1:A:95:GLY:H     | 4        | 0.56          |
| (1,309)  | 1:A:96:ASP:H    | 1:A:95:GLY:H     | 9        | 0.56          |
| (1,308)  | 1:A:96:ASP:H    | 1:A:95:GLY:H     | 6        | 0.56          |
| (1,308)  | 1:A:96:ASP:H    | 1:A:95:GLY:H     | 7        | 0.56          |
| (1,300)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HB2   | 8        | 0.56          |
| (1,300)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HB3   | 8        | 0.56          |
| (1,274)  | 1:A:92:LYS:H    | 1:A:92:LYS:HD2   | 1        | 0.56          |
| (1,274)  | 1:A:92:LYS:H    | 1:A:92:LYS:HD3   | 1        | 0.56          |
| (1,256)  | 1:A:89:LEU:HA   | 1:A:102:GLY:HA2  | 3        | 0.56          |
| (1,255)  | 1:A:89:LEU:HA   | 1:A:102:GLY:HA2  | 3        | 0.56          |
| (1,1762) | 1:A:122:TYR:HB2 | 1:B:111:HIS:H    | 6        | 0.56          |
| (1,1762) | 1:A:122:TYR:HB3 | 1:B:111:HIS:H    | 6        | 0.56          |
| (1,1715) | 1:B:147:GLY:HA3 | 1:B:147:GLY:H    | 9        | 0.56          |
| (1,1665) | 1:B:144:THR:H   | 1:B:143:LEU:HD11 | 4        | 0.56          |
| (1,1665) | 1:B:144:THR:H   | 1:B:143:LEU:HD12 | 4        | 0.56          |
| (1,1665) | 1:B:144:THR:H   | 1:B:143:LEU:HD13 | 4        | 0.56          |
| (1,1665) | 1:B:144:THR:H   | 1:B:143:LEU:HD21 | 4        | 0.56          |
| (1,1665) | 1:B:144:THR:H   | 1:B:143:LEU:HD22 | 4        | 0.56          |
| (1,1665) | 1:B:144:THR:H   | 1:B:143:LEU:HD23 | 4        | 0.56          |
| (1,158)  | 1:A:81:VAL:H    | 1:A:81:VAL:HB    | 5        | 0.56          |
| (1,1541) | 1:B:127:ASP:H   | 1:B:128:VAL:HG11 | 2        | 0.56          |
| (1,1541) | 1:B:127:ASP:H   | 1:B:128:VAL:HG12 | 2        | 0.56          |
| (1,1541) | 1:B:127:ASP:H   | 1:B:128:VAL:HG13 | 2        | 0.56          |
| (1,1541) | 1:B:127:ASP:H   | 1:B:128:VAL:HG21 | 2        | 0.56          |
| (1,1541) | 1:B:127:ASP:H   | 1:B:128:VAL:HG22 | 2        | 0.56          |
| (1,1541) | 1:B:127:ASP:H   | 1:B:128:VAL:HG23 | 2        | 0.56          |
| (1,151)  | 1:A:81:VAL:HG11 | 1:A:79:LEU:HG    | 2        | 0.56          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,151)  | 1:A:81:VAL:HG12 | 1:A:79:LEU:HG   | 2        | 0.56          |
| (1,151)  | 1:A:81:VAL:HG13 | 1:A:79:LEU:HG   | 2        | 0.56          |
| (1,1447) | 1:B:120:ARG:H   | 1:B:100:VAL:H   | 8        | 0.56          |
| (1,1364) | 1:B:113:PHE:HD1 | 1:B:113:PHE:H   | 7        | 0.56          |
| (1,1364) | 1:B:113:PHE:HD2 | 1:B:113:PHE:H   | 7        | 0.56          |
| (1,1348) | 1:B:113:PHE:HA  | 1:B:107:ARG:HB2 | 4        | 0.56          |
| (1,1314) | 1:B:109:ASP:H   | 1:B:109:ASP:HB2 | 6        | 0.56          |
| (1,1314) | 1:B:109:ASP:H   | 1:B:109:ASP:HB3 | 6        | 0.56          |
| (1,1299) | 1:B:107:ARG:HG2 | 1:B:108:GLN:H   | 7        | 0.56          |
| (1,1299) | 1:B:107:ARG:HG3 | 1:B:108:GLN:H   | 7        | 0.56          |
| (1,1254) | 1:B:102:GLY:HA3 | 1:B:102:GLY:H   | 5        | 0.56          |
| (1,1254) | 1:B:102:GLY:HA3 | 1:B:102:GLY:H   | 6        | 0.56          |
| (1,1222) | 1:B:99:GLU:HB2  | 1:B:121:LYS:HG2 | 5        | 0.56          |
| (1,1222) | 1:B:99:GLU:HB2  | 1:B:121:LYS:HG3 | 5        | 0.56          |
| (1,1222) | 1:B:99:GLU:HB3  | 1:B:121:LYS:HG2 | 5        | 0.56          |
| (1,1222) | 1:B:99:GLU:HB3  | 1:B:121:LYS:HG3 | 5        | 0.56          |
| (1,119)  | 1:A:77:VAL:HB   | 1:A:146:ASP:HB3 | 4        | 0.56          |
| (1,1176) | 1:B:96:ASP:H    | 1:B:95:GLY:H    | 4        | 0.56          |
| (1,1176) | 1:B:96:ASP:H    | 1:B:95:GLY:H    | 9        | 0.56          |
| (1,1175) | 1:B:96:ASP:H    | 1:B:95:GLY:H    | 1        | 0.56          |
| (1,1175) | 1:B:96:ASP:H    | 1:B:95:GLY:H    | 6        | 0.56          |
| (1,1175) | 1:B:96:ASP:H    | 1:B:95:GLY:H    | 7        | 0.56          |
| (1,1141) | 1:B:92:LYS:H    | 1:B:92:LYS:HD2  | 1        | 0.56          |
| (1,1141) | 1:B:92:LYS:H    | 1:B:92:LYS:HD3  | 1        | 0.56          |
| (1,1123) | 1:B:89:LEU:HA   | 1:B:102:GLY:HA2 | 3        | 0.56          |
| (1,1122) | 1:B:89:LEU:HA   | 1:B:102:GLY:HA2 | 3        | 0.56          |
| (1,110)  | 1:A:77:VAL:HG11 | 1:A:98:ILE:HD11 | 3        | 0.56          |
| (1,110)  | 1:A:77:VAL:HG11 | 1:A:98:ILE:HD12 | 3        | 0.56          |
| (1,110)  | 1:A:77:VAL:HG11 | 1:A:98:ILE:HD13 | 3        | 0.56          |
| (1,110)  | 1:A:77:VAL:HG12 | 1:A:98:ILE:HD11 | 3        | 0.56          |
| (1,110)  | 1:A:77:VAL:HG12 | 1:A:98:ILE:HD12 | 3        | 0.56          |
| (1,110)  | 1:A:77:VAL:HG12 | 1:A:98:ILE:HD13 | 3        | 0.56          |
| (1,110)  | 1:A:77:VAL:HG13 | 1:A:98:ILE:HD11 | 3        | 0.56          |
| (1,110)  | 1:A:77:VAL:HG13 | 1:A:98:ILE:HD12 | 3        | 0.56          |
| (1,110)  | 1:A:77:VAL:HG13 | 1:A:98:ILE:HD13 | 3        | 0.56          |
| (1,107)  | 1:A:77:VAL:HG11 | 1:A:79:LEU:HG   | 1        | 0.56          |
| (1,107)  | 1:A:77:VAL:HG12 | 1:A:79:LEU:HG   | 1        | 0.56          |
| (1,107)  | 1:A:77:VAL:HG13 | 1:A:79:LEU:HG   | 1        | 0.56          |
| (1,105)  | 1:A:77:VAL:HG21 | 1:A:79:LEU:HG   | 8        | 0.56          |
| (1,105)  | 1:A:77:VAL:HG22 | 1:A:79:LEU:HG   | 8        | 0.56          |
| (1,105)  | 1:A:77:VAL:HG23 | 1:A:79:LEU:HG   | 8        | 0.56          |
| (1,1025) | 1:B:81:VAL:H    | 1:B:81:VAL:HB   | 5        | 0.56          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,981) | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG11 | 5        | 0.55          |
| (1,981) | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG12 | 5        | 0.55          |
| (1,981) | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG13 | 5        | 0.55          |
| (1,981) | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG11 | 5        | 0.55          |
| (1,981) | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG12 | 5        | 0.55          |
| (1,981) | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG13 | 5        | 0.55          |
| (1,981) | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG11 | 5        | 0.55          |
| (1,981) | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG12 | 5        | 0.55          |
| (1,981) | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG13 | 5        | 0.55          |
| (1,978) | 1:B:77:VAL:HG11 | 1:B:122:TYR:HE1  | 1        | 0.55          |
| (1,978) | 1:B:77:VAL:HG11 | 1:B:122:TYR:HE2  | 1        | 0.55          |
| (1,978) | 1:B:77:VAL:HG12 | 1:B:122:TYR:HE1  | 1        | 0.55          |
| (1,978) | 1:B:77:VAL:HG12 | 1:B:122:TYR:HE2  | 1        | 0.55          |
| (1,978) | 1:B:77:VAL:HG13 | 1:B:122:TYR:HE1  | 1        | 0.55          |
| (1,978) | 1:B:77:VAL:HG13 | 1:B:122:TYR:HE2  | 1        | 0.55          |
| (1,972) | 1:B:77:VAL:HG21 | 1:B:79:LEU:HG    | 8        | 0.55          |
| (1,972) | 1:B:77:VAL:HG22 | 1:B:79:LEU:HG    | 8        | 0.55          |
| (1,972) | 1:B:77:VAL:HG23 | 1:B:79:LEU:HG    | 8        | 0.55          |
| (1,964) | 1:B:77:VAL:HG21 | 1:B:77:VAL:H     | 3        | 0.55          |
| (1,964) | 1:B:77:VAL:HG22 | 1:B:77:VAL:H     | 3        | 0.55          |
| (1,964) | 1:B:77:VAL:HG23 | 1:B:77:VAL:H     | 3        | 0.55          |
| (1,954) | 1:B:77:VAL:HG21 | 1:B:75:PHE:HD1   | 6        | 0.55          |
| (1,954) | 1:B:77:VAL:HG21 | 1:B:75:PHE:HD2   | 6        | 0.55          |
| (1,954) | 1:B:77:VAL:HG22 | 1:B:75:PHE:HD1   | 6        | 0.55          |
| (1,954) | 1:B:77:VAL:HG22 | 1:B:75:PHE:HD2   | 6        | 0.55          |
| (1,954) | 1:B:77:VAL:HG23 | 1:B:75:PHE:HD1   | 6        | 0.55          |
| (1,954) | 1:B:77:VAL:HG23 | 1:B:75:PHE:HD2   | 6        | 0.55          |
| (1,917) | 1:B:75:PHE:HD1  | 1:B:75:PHE:H     | 4        | 0.55          |
| (1,917) | 1:B:75:PHE:HD2  | 1:B:75:PHE:H     | 4        | 0.55          |
| (1,87)  | 1:A:77:VAL:HG21 | 1:A:75:PHE:HD1   | 6        | 0.55          |
| (1,87)  | 1:A:77:VAL:HG21 | 1:A:75:PHE:HD2   | 6        | 0.55          |
| (1,87)  | 1:A:77:VAL:HG22 | 1:A:75:PHE:HD1   | 6        | 0.55          |
| (1,87)  | 1:A:77:VAL:HG22 | 1:A:75:PHE:HD2   | 6        | 0.55          |
| (1,87)  | 1:A:77:VAL:HG23 | 1:A:75:PHE:HD1   | 6        | 0.55          |
| (1,87)  | 1:A:77:VAL:HG23 | 1:A:75:PHE:HD2   | 6        | 0.55          |
| (1,848) | 1:A:147:GLY:HA3 | 1:A:147:GLY:H    | 1        | 0.55          |
| (1,841) | 1:A:147:GLY:HA2 | 1:A:132:THR:HA   | 1        | 0.55          |
| (1,840) | 1:A:146:ASP:HA  | 1:A:147:GLY:H    | 2        | 0.55          |
| (1,674) | 1:A:127:ASP:H   | 1:A:128:VAL:HG11 | 1        | 0.55          |
| (1,674) | 1:A:127:ASP:H   | 1:A:128:VAL:HG12 | 1        | 0.55          |
| (1,674) | 1:A:127:ASP:H   | 1:A:128:VAL:HG13 | 1        | 0.55          |
| (1,674) | 1:A:127:ASP:H   | 1:A:128:VAL:HG21 | 1        | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG22 | 1        | 0.55          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG23 | 1        | 0.55          |
| (1,633)  | 1:A:124:ILE:HA   | 1:A:124:ILE:H    | 6        | 0.55          |
| (1,621)  | 1:A:124:ILE:HD11 | 1:A:123:ARG:HA   | 7        | 0.55          |
| (1,621)  | 1:A:124:ILE:HD12 | 1:A:123:ARG:HA   | 7        | 0.55          |
| (1,621)  | 1:A:124:ILE:HD13 | 1:A:123:ARG:HA   | 7        | 0.55          |
| (1,615)  | 1:A:124:ILE:HB   | 1:A:97:VAL:HA    | 2        | 0.55          |
| (1,53)   | 1:A:75:PHE:HE1   | 1:A:133:ILE:HD11 | 1        | 0.55          |
| (1,53)   | 1:A:75:PHE:HE1   | 1:A:133:ILE:HD12 | 1        | 0.55          |
| (1,53)   | 1:A:75:PHE:HE1   | 1:A:133:ILE:HD13 | 1        | 0.55          |
| (1,53)   | 1:A:75:PHE:HE2   | 1:A:133:ILE:HD11 | 1        | 0.55          |
| (1,53)   | 1:A:75:PHE:HE2   | 1:A:133:ILE:HD12 | 1        | 0.55          |
| (1,53)   | 1:A:75:PHE:HE2   | 1:A:133:ILE:HD13 | 1        | 0.55          |
| (1,50)   | 1:A:75:PHE:HD1   | 1:A:75:PHE:H     | 4        | 0.55          |
| (1,50)   | 1:A:75:PHE:HD2   | 1:A:75:PHE:H     | 4        | 0.55          |
| (1,492)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HE1  | 6        | 0.55          |
| (1,492)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HE2  | 6        | 0.55          |
| (1,492)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HE1  | 8        | 0.55          |
| (1,492)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HE2  | 8        | 0.55          |
| (1,330)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA   | 4        | 0.55          |
| (1,329)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA   | 4        | 0.55          |
| (1,308)  | 1:A:96:ASP:H     | 1:A:95:GLY:H     | 1        | 0.55          |
| (1,308)  | 1:A:96:ASP:H     | 1:A:95:GLY:H     | 4        | 0.55          |
| (1,308)  | 1:A:96:ASP:H     | 1:A:95:GLY:H     | 9        | 0.55          |
| (1,216)  | 1:A:85:SER:HB2   | 1:A:89:LEU:H     | 1        | 0.55          |
| (1,192)  | 1:A:84:PHE:HD1   | 1:A:83:HIS:HB3   | 6        | 0.55          |
| (1,192)  | 1:A:84:PHE:HD2   | 1:A:83:HIS:HB3   | 6        | 0.55          |
| (1,173)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HD2   | 8        | 0.55          |
| (1,1715) | 1:B:147:GLY:HA3  | 1:B:147:GLY:H    | 1        | 0.55          |
| (1,1708) | 1:B:147:GLY:HA2  | 1:B:132:THR:HA   | 1        | 0.55          |
| (1,1707) | 1:B:146:ASP:HA   | 1:B:147:GLY:H    | 2        | 0.55          |
| (1,1666) | 1:B:144:THR:HG21 | 1:B:144:THR:HA   | 2        | 0.55          |
| (1,1666) | 1:B:144:THR:HG22 | 1:B:144:THR:HA   | 2        | 0.55          |
| (1,1666) | 1:B:144:THR:HG23 | 1:B:144:THR:HA   | 2        | 0.55          |
| (1,1666) | 1:B:144:THR:HG21 | 1:B:144:THR:HA   | 4        | 0.55          |
| (1,1666) | 1:B:144:THR:HG22 | 1:B:144:THR:HA   | 4        | 0.55          |
| (1,1666) | 1:B:144:THR:HG23 | 1:B:144:THR:HA   | 4        | 0.55          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG11 | 1        | 0.55          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG12 | 1        | 0.55          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG13 | 1        | 0.55          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG21 | 1        | 0.55          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG22 | 1        | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG23 | 1        | 0.55          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG11 | 9        | 0.55          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG12 | 9        | 0.55          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG13 | 9        | 0.55          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG21 | 9        | 0.55          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG22 | 9        | 0.55          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG23 | 9        | 0.55          |
| (1,1500) | 1:B:124:ILE:HA   | 1:B:124:ILE:H    | 6        | 0.55          |
| (1,1488) | 1:B:124:ILE:HD11 | 1:B:123:ARG:HA   | 7        | 0.55          |
| (1,1488) | 1:B:124:ILE:HD12 | 1:B:123:ARG:HA   | 7        | 0.55          |
| (1,1488) | 1:B:124:ILE:HD13 | 1:B:123:ARG:HA   | 7        | 0.55          |
| (1,1482) | 1:B:124:ILE:HB   | 1:B:97:VAL:HA    | 2        | 0.55          |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE1  | 6        | 0.55          |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE2  | 6        | 0.55          |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE1  | 8        | 0.55          |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE2  | 8        | 0.55          |
| (1,1310) | 1:B:108:GLN:HA   | 1:B:109:ASP:H    | 1        | 0.55          |
| (1,1254) | 1:B:102:GLY:HA3  | 1:B:102:GLY:H    | 8        | 0.55          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG21 | 4        | 0.55          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG22 | 4        | 0.55          |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG23 | 4        | 0.55          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG21 | 4        | 0.55          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG22 | 4        | 0.55          |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG23 | 4        | 0.55          |
| (1,1175) | 1:B:96:ASP:H     | 1:B:95:GLY:H     | 4        | 0.55          |
| (1,1175) | 1:B:96:ASP:H     | 1:B:95:GLY:H     | 9        | 0.55          |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB2   | 8        | 0.55          |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB3   | 8        | 0.55          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG11 | 5        | 0.55          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG12 | 5        | 0.55          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG13 | 5        | 0.55          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG11 | 5        | 0.55          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG12 | 5        | 0.55          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG13 | 5        | 0.55          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG11 | 5        | 0.55          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG12 | 5        | 0.55          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG13 | 5        | 0.55          |
| (1,111)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HE1  | 1        | 0.55          |
| (1,111)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HE2  | 1        | 0.55          |
| (1,111)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HE1  | 1        | 0.55          |
| (1,111)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HE2  | 1        | 0.55          |
| (1,111)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HE1  | 1        | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,111)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HE2  | 1        | 0.55          |
| (1,1083) | 1:B:85:SER:HB2   | 1:B:89:LEU:H     | 1        | 0.55          |
| (1,1059) | 1:B:84:PHE:HD1   | 1:B:83:HIS:HB3   | 6        | 0.55          |
| (1,1059) | 1:B:84:PHE:HD2   | 1:B:83:HIS:HB3   | 6        | 0.55          |
| (1,1040) | 1:B:83:HIS:HA    | 1:B:83:HIS:HD2   | 8        | 0.55          |
| (1,976)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:H     | 4        | 0.54          |
| (1,976)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:H     | 4        | 0.54          |
| (1,976)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:H     | 4        | 0.54          |
| (1,920)  | 1:B:75:PHE:HE1   | 1:B:133:ILE:HD11 | 1        | 0.54          |
| (1,920)  | 1:B:75:PHE:HE1   | 1:B:133:ILE:HD12 | 1        | 0.54          |
| (1,920)  | 1:B:75:PHE:HE1   | 1:B:133:ILE:HD13 | 1        | 0.54          |
| (1,920)  | 1:B:75:PHE:HE2   | 1:B:133:ILE:HD11 | 1        | 0.54          |
| (1,920)  | 1:B:75:PHE:HE2   | 1:B:133:ILE:HD12 | 1        | 0.54          |
| (1,920)  | 1:B:75:PHE:HE2   | 1:B:133:ILE:HD13 | 1        | 0.54          |
| (1,886)  | 1:B:70:LEU:HD11  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,886)  | 1:B:70:LEU:HD12  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,886)  | 1:B:70:LEU:HD13  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,886)  | 1:B:70:LEU:HD21  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,886)  | 1:B:70:LEU:HD22  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,886)  | 1:B:70:LEU:HD23  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,885)  | 1:B:70:LEU:HD11  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,885)  | 1:B:70:LEU:HD12  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,885)  | 1:B:70:LEU:HD13  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,885)  | 1:B:70:LEU:HD21  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,885)  | 1:B:70:LEU:HD22  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,885)  | 1:B:70:LEU:HD23  | 1:B:70:LEU:H     | 8        | 0.54          |
| (1,871)  | 1:B:66:SER:HA    | 1:B:79:LEU:HD11  | 1        | 0.54          |
| (1,871)  | 1:B:66:SER:HA    | 1:B:79:LEU:HD12  | 1        | 0.54          |
| (1,871)  | 1:B:66:SER:HA    | 1:B:79:LEU:HD13  | 1        | 0.54          |
| (1,871)  | 1:B:66:SER:HA    | 1:B:79:LEU:HD21  | 1        | 0.54          |
| (1,871)  | 1:B:66:SER:HA    | 1:B:79:LEU:HD22  | 1        | 0.54          |
| (1,871)  | 1:B:66:SER:HA    | 1:B:79:LEU:HD23  | 1        | 0.54          |
| (1,848)  | 1:A:147:GLY:HA3  | 1:A:147:GLY:H    | 6        | 0.54          |
| (1,799)  | 1:A:144:THR:HG21 | 1:A:144:THR:HA   | 2        | 0.54          |
| (1,799)  | 1:A:144:THR:HG22 | 1:A:144:THR:HA   | 2        | 0.54          |
| (1,799)  | 1:A:144:THR:HG23 | 1:A:144:THR:HA   | 2        | 0.54          |
| (1,799)  | 1:A:144:THR:HG21 | 1:A:144:THR:HA   | 4        | 0.54          |
| (1,799)  | 1:A:144:THR:HG22 | 1:A:144:THR:HA   | 4        | 0.54          |
| (1,799)  | 1:A:144:THR:HG23 | 1:A:144:THR:HA   | 4        | 0.54          |
| (1,799)  | 1:A:144:THR:HG21 | 1:A:144:THR:HA   | 7        | 0.54          |
| (1,799)  | 1:A:144:THR:HG22 | 1:A:144:THR:HA   | 7        | 0.54          |
| (1,799)  | 1:A:144:THR:HG23 | 1:A:144:THR:HA   | 7        | 0.54          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,700) | 1:A:132:THR:HG21 | 1:A:132:THR:H    | 5        | 0.54          |
| (1,700) | 1:A:132:THR:HG22 | 1:A:132:THR:H    | 5        | 0.54          |
| (1,700) | 1:A:132:THR:HG23 | 1:A:132:THR:H    | 5        | 0.54          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG11 | 9        | 0.54          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG12 | 9        | 0.54          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG13 | 9        | 0.54          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG21 | 9        | 0.54          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG22 | 9        | 0.54          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG23 | 9        | 0.54          |
| (1,633) | 1:A:124:ILE:HA   | 1:A:124:ILE:H    | 9        | 0.54          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG11  | 9        | 0.54          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG12  | 9        | 0.54          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG13  | 9        | 0.54          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG21  | 9        | 0.54          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG22  | 9        | 0.54          |
| (1,604) | 1:A:123:ARG:HB2  | 1:A:97:VAL:HG23  | 9        | 0.54          |
| (1,590) | 1:A:122:TYR:HA   | 1:A:98:ILE:H     | 6        | 0.54          |
| (1,569) | 1:A:119:HIS:HA   | 1:A:101:HIS:HA   | 9        | 0.54          |
| (1,548) | 1:A:117:GLU:HA   | 1:A:118:PHE:H    | 3        | 0.54          |
| (1,497) | 1:A:113:PHE:HD1  | 1:A:113:PHE:H    | 8        | 0.54          |
| (1,497) | 1:A:113:PHE:HD2  | 1:A:113:PHE:H    | 8        | 0.54          |
| (1,492) | 1:A:113:PHE:HA   | 1:A:113:PHE:HE1  | 5        | 0.54          |
| (1,492) | 1:A:113:PHE:HA   | 1:A:113:PHE:HE2  | 5        | 0.54          |
| (1,451) | 1:A:109:ASP:H    | 1:A:112:GLY:H    | 7        | 0.54          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD11  | 1        | 0.54          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD12  | 1        | 0.54          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD13  | 1        | 0.54          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD21  | 1        | 0.54          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD22  | 1        | 0.54          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD23  | 1        | 0.54          |
| (1,387) | 1:A:102:GLY:HA3  | 1:A:102:GLY:H    | 8        | 0.54          |
| (1,291) | 1:A:94:LEU:HD11  | 1:A:94:LEU:H     | 9        | 0.54          |
| (1,291) | 1:A:94:LEU:HD12  | 1:A:94:LEU:H     | 9        | 0.54          |
| (1,291) | 1:A:94:LEU:HD13  | 1:A:94:LEU:H     | 9        | 0.54          |
| (1,291) | 1:A:94:LEU:HD21  | 1:A:94:LEU:H     | 9        | 0.54          |
| (1,291) | 1:A:94:LEU:HD22  | 1:A:94:LEU:H     | 9        | 0.54          |
| (1,291) | 1:A:94:LEU:HD23  | 1:A:94:LEU:H     | 9        | 0.54          |
| (1,271) | 1:A:91:VAL:HB    | 1:A:92:LYS:H     | 5        | 0.54          |
| (1,193) | 1:A:84:PHE:HD1   | 1:A:83:HIS:HA    | 6        | 0.54          |
| (1,193) | 1:A:84:PHE:HD2   | 1:A:83:HIS:HA    | 6        | 0.54          |
| (1,19)  | 1:A:70:LEU:HD11  | 1:A:70:LEU:H     | 8        | 0.54          |
| (1,19)  | 1:A:70:LEU:HD12  | 1:A:70:LEU:H     | 8        | 0.54          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,19)   | 1:A:70:LEU:HD13  | 1:A:70:LEU:H    | 8        | 0.54          |
| (1,19)   | 1:A:70:LEU:HD21  | 1:A:70:LEU:H    | 8        | 0.54          |
| (1,19)   | 1:A:70:LEU:HD22  | 1:A:70:LEU:H    | 8        | 0.54          |
| (1,19)   | 1:A:70:LEU:HD23  | 1:A:70:LEU:H    | 8        | 0.54          |
| (1,18)   | 1:A:70:LEU:HD11  | 1:A:70:LEU:H    | 8        | 0.54          |
| (1,18)   | 1:A:70:LEU:HD12  | 1:A:70:LEU:H    | 8        | 0.54          |
| (1,18)   | 1:A:70:LEU:HD13  | 1:A:70:LEU:H    | 8        | 0.54          |
| (1,18)   | 1:A:70:LEU:HD21  | 1:A:70:LEU:H    | 8        | 0.54          |
| (1,18)   | 1:A:70:LEU:HD22  | 1:A:70:LEU:H    | 8        | 0.54          |
| (1,18)   | 1:A:70:LEU:HD23  | 1:A:70:LEU:H    | 8        | 0.54          |
| (1,173)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HD2  | 2        | 0.54          |
| (1,1715) | 1:B:147:GLY:HA3  | 1:B:147:GLY:H   | 6        | 0.54          |
| (1,1666) | 1:B:144:THR:HG21 | 1:B:144:THR:HA  | 3        | 0.54          |
| (1,1666) | 1:B:144:THR:HG22 | 1:B:144:THR:HA  | 3        | 0.54          |
| (1,1666) | 1:B:144:THR:HG23 | 1:B:144:THR:HA  | 3        | 0.54          |
| (1,1666) | 1:B:144:THR:HG21 | 1:B:144:THR:HA  | 7        | 0.54          |
| (1,1666) | 1:B:144:THR:HG22 | 1:B:144:THR:HA  | 7        | 0.54          |
| (1,1666) | 1:B:144:THR:HG23 | 1:B:144:THR:HA  | 7        | 0.54          |
| (1,158)  | 1:A:81:VAL:H     | 1:A:81:VAL:HB   | 3        | 0.54          |
| (1,1567) | 1:B:132:THR:HG21 | 1:B:132:THR:H   | 5        | 0.54          |
| (1,1567) | 1:B:132:THR:HG22 | 1:B:132:THR:H   | 5        | 0.54          |
| (1,1567) | 1:B:132:THR:HG23 | 1:B:132:THR:H   | 5        | 0.54          |
| (1,155)  | 1:A:81:VAL:HG11  | 1:A:81:VAL:HA   | 1        | 0.54          |
| (1,155)  | 1:A:81:VAL:HG12  | 1:A:81:VAL:HA   | 1        | 0.54          |
| (1,155)  | 1:A:81:VAL:HG13  | 1:A:81:VAL:HA   | 1        | 0.54          |
| (1,153)  | 1:A:81:VAL:HG11  | 1:A:80:ASP:HA   | 4        | 0.54          |
| (1,153)  | 1:A:81:VAL:HG12  | 1:A:80:ASP:HA   | 4        | 0.54          |
| (1,153)  | 1:A:81:VAL:HG13  | 1:A:80:ASP:HA   | 4        | 0.54          |
| (1,153)  | 1:A:81:VAL:HG11  | 1:A:80:ASP:HA   | 7        | 0.54          |
| (1,153)  | 1:A:81:VAL:HG12  | 1:A:80:ASP:HA   | 7        | 0.54          |
| (1,153)  | 1:A:81:VAL:HG13  | 1:A:80:ASP:HA   | 7        | 0.54          |
| (1,1500) | 1:B:124:ILE:HA   | 1:B:124:ILE:H   | 9        | 0.54          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG11 | 9        | 0.54          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG12 | 9        | 0.54          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG13 | 9        | 0.54          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG21 | 9        | 0.54          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG22 | 9        | 0.54          |
| (1,1471) | 1:B:123:ARG:HB2  | 1:B:97:VAL:HG23 | 9        | 0.54          |
| (1,1457) | 1:B:122:TYR:HA   | 1:B:98:ILE:H    | 6        | 0.54          |
| (1,1436) | 1:B:119:HIS:HA   | 1:B:101:HIS:HA  | 9        | 0.54          |
| (1,1415) | 1:B:117:GLU:HA   | 1:B:118:PHE:H   | 3        | 0.54          |
| (1,1364) | 1:B:113:PHE:HD1  | 1:B:113:PHE:H   | 8        | 0.54          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1364) | 1:B:113:PHE:HD2  | 1:B:113:PHE:H   | 8        | 0.54          |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE1 | 5        | 0.54          |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE2 | 5        | 0.54          |
| (1,1318) | 1:B:109:ASP:H    | 1:B:112:GLY:H   | 7        | 0.54          |
| (1,1197) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 4        | 0.54          |
| (1,1196) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 4        | 0.54          |
| (1,1158) | 1:B:94:LEU:HD11  | 1:B:94:LEU:H    | 9        | 0.54          |
| (1,1158) | 1:B:94:LEU:HD12  | 1:B:94:LEU:H    | 9        | 0.54          |
| (1,1158) | 1:B:94:LEU:HD13  | 1:B:94:LEU:H    | 9        | 0.54          |
| (1,1158) | 1:B:94:LEU:HD21  | 1:B:94:LEU:H    | 9        | 0.54          |
| (1,1158) | 1:B:94:LEU:HD22  | 1:B:94:LEU:H    | 9        | 0.54          |
| (1,1158) | 1:B:94:LEU:HD23  | 1:B:94:LEU:H    | 9        | 0.54          |
| (1,1138) | 1:B:91:VAL:HB    | 1:B:92:LYS:H    | 5        | 0.54          |
| (1,109)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:H    | 4        | 0.54          |
| (1,109)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:H    | 4        | 0.54          |
| (1,109)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:H    | 4        | 0.54          |
| (1,1060) | 1:B:84:PHE:HD1   | 1:B:83:HIS:HA   | 6        | 0.54          |
| (1,1060) | 1:B:84:PHE:HD2   | 1:B:83:HIS:HA   | 6        | 0.54          |
| (1,1051) | 1:B:83:HIS:H     | 1:B:84:PHE:H    | 9        | 0.54          |
| (1,1050) | 1:B:83:HIS:H     | 1:B:84:PHE:H    | 9        | 0.54          |
| (1,1040) | 1:B:83:HIS:HA    | 1:B:83:HIS:HD2  | 2        | 0.54          |
| (1,1025) | 1:B:81:VAL:H     | 1:B:81:VAL:HB   | 3        | 0.54          |
| (1,1022) | 1:B:81:VAL:HG11  | 1:B:81:VAL:HA   | 1        | 0.54          |
| (1,1022) | 1:B:81:VAL:HG12  | 1:B:81:VAL:HA   | 1        | 0.54          |
| (1,1022) | 1:B:81:VAL:HG13  | 1:B:81:VAL:HA   | 1        | 0.54          |
| (1,1020) | 1:B:81:VAL:HG11  | 1:B:80:ASP:HA   | 4        | 0.54          |
| (1,1020) | 1:B:81:VAL:HG12  | 1:B:80:ASP:HA   | 4        | 0.54          |
| (1,1020) | 1:B:81:VAL:HG13  | 1:B:80:ASP:HA   | 4        | 0.54          |
| (1,1020) | 1:B:81:VAL:HG11  | 1:B:80:ASP:HA   | 7        | 0.54          |
| (1,1020) | 1:B:81:VAL:HG12  | 1:B:80:ASP:HA   | 7        | 0.54          |
| (1,1020) | 1:B:81:VAL:HG13  | 1:B:80:ASP:HA   | 7        | 0.54          |
| (1,97)   | 1:A:77:VAL:HG21  | 1:A:77:VAL:H    | 7        | 0.53          |
| (1,97)   | 1:A:77:VAL:HG22  | 1:A:77:VAL:H    | 7        | 0.53          |
| (1,97)   | 1:A:77:VAL:HG23  | 1:A:77:VAL:H    | 7        | 0.53          |
| (1,964)  | 1:B:77:VAL:HG21  | 1:B:77:VAL:H    | 7        | 0.53          |
| (1,964)  | 1:B:77:VAL:HG22  | 1:B:77:VAL:H    | 7        | 0.53          |
| (1,964)  | 1:B:77:VAL:HG23  | 1:B:77:VAL:H    | 7        | 0.53          |
| (1,799)  | 1:A:144:THR:HG21 | 1:A:144:THR:HA  | 3        | 0.53          |
| (1,799)  | 1:A:144:THR:HG22 | 1:A:144:THR:HA  | 3        | 0.53          |
| (1,799)  | 1:A:144:THR:HG23 | 1:A:144:THR:HA  | 3        | 0.53          |
| (1,799)  | 1:A:144:THR:HG21 | 1:A:144:THR:HA  | 8        | 0.53          |
| (1,799)  | 1:A:144:THR:HG22 | 1:A:144:THR:HA  | 8        | 0.53          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,799) | 1:A:144:THR:HG23 | 1:A:144:THR:HA   | 8        | 0.53          |
| (1,799) | 1:A:144:THR:HG21 | 1:A:144:THR:HA   | 9        | 0.53          |
| (1,799) | 1:A:144:THR:HG22 | 1:A:144:THR:HA   | 9        | 0.53          |
| (1,799) | 1:A:144:THR:HG23 | 1:A:144:THR:HA   | 9        | 0.53          |
| (1,798) | 1:A:144:THR:H    | 1:A:143:LEU:HD11 | 7        | 0.53          |
| (1,798) | 1:A:144:THR:H    | 1:A:143:LEU:HD12 | 7        | 0.53          |
| (1,798) | 1:A:144:THR:H    | 1:A:143:LEU:HD13 | 7        | 0.53          |
| (1,798) | 1:A:144:THR:H    | 1:A:143:LEU:HD21 | 7        | 0.53          |
| (1,798) | 1:A:144:THR:H    | 1:A:143:LEU:HD22 | 7        | 0.53          |
| (1,798) | 1:A:144:THR:H    | 1:A:143:LEU:HD23 | 7        | 0.53          |
| (1,750) | 1:A:136:SER:H    | 1:A:143:LEU:HD11 | 2        | 0.53          |
| (1,750) | 1:A:136:SER:H    | 1:A:143:LEU:HD12 | 2        | 0.53          |
| (1,750) | 1:A:136:SER:H    | 1:A:143:LEU:HD13 | 2        | 0.53          |
| (1,750) | 1:A:136:SER:H    | 1:A:143:LEU:HD21 | 2        | 0.53          |
| (1,750) | 1:A:136:SER:H    | 1:A:143:LEU:HD22 | 2        | 0.53          |
| (1,750) | 1:A:136:SER:H    | 1:A:143:LEU:HD23 | 2        | 0.53          |
| (1,633) | 1:A:124:ILE:HA   | 1:A:124:ILE:H    | 7        | 0.53          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB2  | 5        | 0.53          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB3  | 5        | 0.53          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB2  | 6        | 0.53          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB3  | 6        | 0.53          |
| (1,583) | 1:A:121:LYS:HA   | 1:A:99:GLU:HA    | 5        | 0.53          |
| (1,562) | 1:A:118:PHE:HA   | 1:A:118:PHE:H    | 8        | 0.53          |
| (1,538) | 1:A:116:ARG:H    | 1:A:116:ARG:HB2  | 3        | 0.53          |
| (1,538) | 1:A:116:ARG:H    | 1:A:116:ARG:HB3  | 3        | 0.53          |
| (1,492) | 1:A:113:PHE:HA   | 1:A:113:PHE:HE1  | 2        | 0.53          |
| (1,492) | 1:A:113:PHE:HA   | 1:A:113:PHE:HE2  | 2        | 0.53          |
| (1,470) | 1:A:111:HIS:HA   | 1:A:112:GLY:H    | 1        | 0.53          |
| (1,432) | 1:A:107:ARG:HG2  | 1:A:108:GLN:H    | 2        | 0.53          |
| (1,432) | 1:A:107:ARG:HG3  | 1:A:108:GLN:H    | 2        | 0.53          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG21 | 4        | 0.53          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG22 | 4        | 0.53          |
| (1,352) | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG23 | 4        | 0.53          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG21 | 4        | 0.53          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG22 | 4        | 0.53          |
| (1,352) | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG23 | 4        | 0.53          |
| (1,281) | 1:A:92:LYS:H     | 1:A:101:HIS:H    | 7        | 0.53          |
| (1,271) | 1:A:91:VAL:HB    | 1:A:92:LYS:H     | 9        | 0.53          |
| (1,240) | 1:A:89:LEU:H     | 1:A:88:GLU:HG2   | 9        | 0.53          |
| (1,240) | 1:A:89:LEU:H     | 1:A:88:GLU:HG3   | 9        | 0.53          |
| (1,193) | 1:A:84:PHE:HD1   | 1:A:83:HIS:HA    | 8        | 0.53          |
| (1,193) | 1:A:84:PHE:HD2   | 1:A:83:HIS:HA    | 8        | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,184)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 9        | 0.53          |
| (1,183)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 9        | 0.53          |
| (1,1760) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H    | 8        | 0.53          |
| (1,1760) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H    | 8        | 0.53          |
| (1,173)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HD2   | 4        | 0.53          |
| (1,167)  | 1:A:81:VAL:H     | 1:A:141:GLY:HA2  | 1        | 0.53          |
| (1,1666) | 1:B:144:THR:HG21 | 1:B:144:THR:HA   | 8        | 0.53          |
| (1,1666) | 1:B:144:THR:HG22 | 1:B:144:THR:HA   | 8        | 0.53          |
| (1,1666) | 1:B:144:THR:HG23 | 1:B:144:THR:HA   | 8        | 0.53          |
| (1,1666) | 1:B:144:THR:HG21 | 1:B:144:THR:HA   | 9        | 0.53          |
| (1,1666) | 1:B:144:THR:HG22 | 1:B:144:THR:HA   | 9        | 0.53          |
| (1,1666) | 1:B:144:THR:HG23 | 1:B:144:THR:HA   | 9        | 0.53          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD11 | 7        | 0.53          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD12 | 7        | 0.53          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD13 | 7        | 0.53          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD21 | 7        | 0.53          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD22 | 7        | 0.53          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD23 | 7        | 0.53          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD11 | 2        | 0.53          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD12 | 2        | 0.53          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD13 | 2        | 0.53          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD21 | 2        | 0.53          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD22 | 2        | 0.53          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD23 | 2        | 0.53          |
| (1,1581) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HA   | 2        | 0.53          |
| (1,1581) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HA   | 2        | 0.53          |
| (1,1581) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HA   | 2        | 0.53          |
| (1,1553) | 1:B:129:ASP:H    | 1:B:132:THR:HG1  | 8        | 0.53          |
| (1,155)  | 1:A:81:VAL:HG11  | 1:A:81:VAL:HA    | 2        | 0.53          |
| (1,155)  | 1:A:81:VAL:HG12  | 1:A:81:VAL:HA    | 2        | 0.53          |
| (1,155)  | 1:A:81:VAL:HG13  | 1:A:81:VAL:HA    | 2        | 0.53          |
| (1,1500) | 1:B:124:ILE:HA   | 1:B:124:ILE:H    | 7        | 0.53          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB2  | 5        | 0.53          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB3  | 5        | 0.53          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB2  | 6        | 0.53          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB3  | 6        | 0.53          |
| (1,1450) | 1:B:121:LYS:HA   | 1:B:99:GLU:HA    | 5        | 0.53          |
| (1,1429) | 1:B:118:PHE:HA   | 1:B:118:PHE:H    | 8        | 0.53          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB2  | 3        | 0.53          |
| (1,1405) | 1:B:116:ARG:H    | 1:B:116:ARG:HB3  | 3        | 0.53          |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE1  | 2        | 0.53          |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE2  | 2        | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1337) | 1:B:111:HIS:HA   | 1:B:112:GLY:H    | 1        | 0.53          |
| (1,1299) | 1:B:107:ARG:HG2  | 1:B:108:GLN:H    | 2        | 0.53          |
| (1,1299) | 1:B:107:ARG:HG3  | 1:B:108:GLN:H    | 2        | 0.53          |
| (1,1221) | 1:B:99:GLU:HA    | 1:B:100:VAL:H    | 3        | 0.53          |
| (1,1148) | 1:B:92:LYS:H     | 1:B:101:HIS:H    | 7        | 0.53          |
| (1,1138) | 1:B:91:VAL:HB    | 1:B:92:LYS:H     | 9        | 0.53          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG2   | 9        | 0.53          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG3   | 9        | 0.53          |
| (1,1060) | 1:B:84:PHE:HD1   | 1:B:83:HIS:HA    | 8        | 0.53          |
| (1,1060) | 1:B:84:PHE:HD2   | 1:B:83:HIS:HA    | 8        | 0.53          |
| (1,1040) | 1:B:83:HIS:HA    | 1:B:83:HIS:HD2   | 4        | 0.53          |
| (1,1034) | 1:B:81:VAL:H     | 1:B:141:GLY:HA2  | 1        | 0.53          |
| (1,893)  | 1:B:71:GLU:H     | 1:B:76:SER:H     | 9        | 0.52          |
| (1,840)  | 1:A:146:ASP:HA   | 1:A:147:GLY:H    | 3        | 0.52          |
| (1,799)  | 1:A:144:THR:HG21 | 1:A:144:THR:HA   | 1        | 0.52          |
| (1,799)  | 1:A:144:THR:HG22 | 1:A:144:THR:HA   | 1        | 0.52          |
| (1,799)  | 1:A:144:THR:HG23 | 1:A:144:THR:HA   | 1        | 0.52          |
| (1,783)  | 1:A:142:VAL:HG11 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,783)  | 1:A:142:VAL:HG12 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,783)  | 1:A:142:VAL:HG13 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,783)  | 1:A:142:VAL:HG21 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,783)  | 1:A:142:VAL:HG22 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,783)  | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,782)  | 1:A:142:VAL:HG11 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,782)  | 1:A:142:VAL:HG12 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,782)  | 1:A:142:VAL:HG13 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,782)  | 1:A:142:VAL:HG21 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,782)  | 1:A:142:VAL:HG22 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,782)  | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 5        | 0.52          |
| (1,738)  | 1:A:135:SER:HA   | 1:A:145:VAL:HG21 | 5        | 0.52          |
| (1,738)  | 1:A:135:SER:HA   | 1:A:145:VAL:HG22 | 5        | 0.52          |
| (1,738)  | 1:A:135:SER:HA   | 1:A:145:VAL:HG23 | 5        | 0.52          |
| (1,714)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HA   | 2        | 0.52          |
| (1,714)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HA   | 2        | 0.52          |
| (1,714)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HA   | 2        | 0.52          |
| (1,566)  | 1:A:118:PHE:HA   | 1:A:119:HIS:H    | 5        | 0.52          |
| (1,544)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 5        | 0.52          |
| (1,543)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 5        | 0.52          |
| (1,512)  | 1:A:114:ILE:HD11 | 1:A:113:PHE:HA   | 1        | 0.52          |
| (1,512)  | 1:A:114:ILE:HD12 | 1:A:113:PHE:HA   | 1        | 0.52          |
| (1,512)  | 1:A:114:ILE:HD13 | 1:A:113:PHE:HA   | 1        | 0.52          |
| (1,451)  | 1:A:109:ASP:H    | 1:A:112:GLY:H    | 1        | 0.52          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,354)  | 1:A:99:GLU:HA    | 1:A:100:VAL:H   | 3        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD11  | 1:A:94:LEU:H    | 4        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD12  | 1:A:94:LEU:H    | 4        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD13  | 1:A:94:LEU:H    | 4        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD21  | 1:A:94:LEU:H    | 4        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD22  | 1:A:94:LEU:H    | 4        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD23  | 1:A:94:LEU:H    | 4        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD11  | 1:A:94:LEU:H    | 5        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD12  | 1:A:94:LEU:H    | 5        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD13  | 1:A:94:LEU:H    | 5        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD21  | 1:A:94:LEU:H    | 5        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD22  | 1:A:94:LEU:H    | 5        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD23  | 1:A:94:LEU:H    | 5        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD11  | 1:A:94:LEU:H    | 6        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD12  | 1:A:94:LEU:H    | 6        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD13  | 1:A:94:LEU:H    | 6        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD21  | 1:A:94:LEU:H    | 6        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD22  | 1:A:94:LEU:H    | 6        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD23  | 1:A:94:LEU:H    | 6        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD11  | 1:A:94:LEU:H    | 7        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD12  | 1:A:94:LEU:H    | 7        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD13  | 1:A:94:LEU:H    | 7        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD21  | 1:A:94:LEU:H    | 7        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD22  | 1:A:94:LEU:H    | 7        | 0.52          |
| (1,291)  | 1:A:94:LEU:HD23  | 1:A:94:LEU:H    | 7        | 0.52          |
| (1,271)  | 1:A:91:VAL:HB    | 1:A:92:LYS:H    | 6        | 0.52          |
| (1,260)  | 1:A:89:LEU:HD21  | 1:A:103:LYS:H   | 1        | 0.52          |
| (1,260)  | 1:A:89:LEU:HD22  | 1:A:103:LYS:H   | 1        | 0.52          |
| (1,260)  | 1:A:89:LEU:HD23  | 1:A:103:LYS:H   | 1        | 0.52          |
| (1,26)   | 1:A:71:GLU:H     | 1:A:76:SER:H    | 9        | 0.52          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG2  | 2        | 0.52          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG3  | 2        | 0.52          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG2  | 7        | 0.52          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG3  | 7        | 0.52          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD21 | 8        | 0.52          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD22 | 8        | 0.52          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD23 | 8        | 0.52          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD21 | 8        | 0.52          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD22 | 8        | 0.52          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD23 | 8        | 0.52          |
| (1,1707) | 1:B:146:ASP:HA   | 1:B:147:GLY:H   | 3        | 0.52          |
| (1,1666) | 1:B:144:THR:HG21 | 1:B:144:THR:HA  | 1        | 0.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1666) | 1:B:144:THR:HG22 | 1:B:144:THR:HA   | 1        | 0.52          |
| (1,1666) | 1:B:144:THR:HG23 | 1:B:144:THR:HA   | 1        | 0.52          |
| (1,1650) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1650) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1650) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1650) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1650) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1650) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1649) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1649) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1649) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1649) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1649) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1649) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H    | 5        | 0.52          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG21 | 5        | 0.52          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG22 | 5        | 0.52          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG23 | 5        | 0.52          |
| (1,157)  | 1:A:81:VAL:HG21  | 1:A:81:VAL:H     | 3        | 0.52          |
| (1,157)  | 1:A:81:VAL:HG22  | 1:A:81:VAL:H     | 3        | 0.52          |
| (1,157)  | 1:A:81:VAL:HG23  | 1:A:81:VAL:H     | 3        | 0.52          |
| (1,1436) | 1:B:119:HIS:HA   | 1:B:101:HIS:HA   | 5        | 0.52          |
| (1,1433) | 1:B:118:PHE:HA   | 1:B:119:HIS:H    | 5        | 0.52          |
| (1,1411) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA   | 5        | 0.52          |
| (1,1410) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA   | 5        | 0.52          |
| (1,1407) | 1:B:116:ARG:HA   | 1:B:117:GLU:H    | 5        | 0.52          |
| (1,1379) | 1:B:114:ILE:HD11 | 1:B:113:PHE:HA   | 1        | 0.52          |
| (1,1379) | 1:B:114:ILE:HD12 | 1:B:113:PHE:HA   | 1        | 0.52          |
| (1,1379) | 1:B:114:ILE:HD13 | 1:B:113:PHE:HA   | 1        | 0.52          |
| (1,1318) | 1:B:109:ASP:H    | 1:B:112:GLY:H    | 1        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD11  | 1:B:94:LEU:H     | 4        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD12  | 1:B:94:LEU:H     | 4        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD13  | 1:B:94:LEU:H     | 4        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD21  | 1:B:94:LEU:H     | 4        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD22  | 1:B:94:LEU:H     | 4        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD23  | 1:B:94:LEU:H     | 4        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD11  | 1:B:94:LEU:H     | 5        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD12  | 1:B:94:LEU:H     | 5        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD13  | 1:B:94:LEU:H     | 5        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD21  | 1:B:94:LEU:H     | 5        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD22  | 1:B:94:LEU:H     | 5        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD23  | 1:B:94:LEU:H     | 5        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD11  | 1:B:94:LEU:H     | 6        | 0.52          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1158) | 1:B:94:LEU:HD12 | 1:B:94:LEU:H     | 6        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD13 | 1:B:94:LEU:H     | 6        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD21 | 1:B:94:LEU:H     | 6        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD22 | 1:B:94:LEU:H     | 6        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD23 | 1:B:94:LEU:H     | 6        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD11 | 1:B:94:LEU:H     | 7        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD12 | 1:B:94:LEU:H     | 7        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD13 | 1:B:94:LEU:H     | 7        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD21 | 1:B:94:LEU:H     | 7        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD22 | 1:B:94:LEU:H     | 7        | 0.52          |
| (1,1158) | 1:B:94:LEU:HD23 | 1:B:94:LEU:H     | 7        | 0.52          |
| (1,1138) | 1:B:91:VAL:HB   | 1:B:92:LYS:H     | 6        | 0.52          |
| (1,1127) | 1:B:89:LEU:HD21 | 1:B:103:LYS:H    | 1        | 0.52          |
| (1,1127) | 1:B:89:LEU:HD22 | 1:B:103:LYS:H    | 1        | 0.52          |
| (1,1127) | 1:B:89:LEU:HD23 | 1:B:103:LYS:H    | 1        | 0.52          |
| (1,1107) | 1:B:89:LEU:H    | 1:B:88:GLU:HG2   | 7        | 0.52          |
| (1,1107) | 1:B:89:LEU:H    | 1:B:88:GLU:HG3   | 7        | 0.52          |
| (1,1086) | 1:B:86:PRO:HB2  | 1:B:89:LEU:HD21  | 8        | 0.52          |
| (1,1086) | 1:B:86:PRO:HB2  | 1:B:89:LEU:HD22  | 8        | 0.52          |
| (1,1086) | 1:B:86:PRO:HB2  | 1:B:89:LEU:HD23  | 8        | 0.52          |
| (1,1086) | 1:B:86:PRO:HB3  | 1:B:89:LEU:HD21  | 8        | 0.52          |
| (1,1086) | 1:B:86:PRO:HB3  | 1:B:89:LEU:HD22  | 8        | 0.52          |
| (1,1086) | 1:B:86:PRO:HB3  | 1:B:89:LEU:HD23  | 8        | 0.52          |
| (1,1024) | 1:B:81:VAL:HG21 | 1:B:81:VAL:H     | 3        | 0.52          |
| (1,1024) | 1:B:81:VAL:HG22 | 1:B:81:VAL:H     | 3        | 0.52          |
| (1,1024) | 1:B:81:VAL:HG23 | 1:B:81:VAL:H     | 3        | 0.52          |
| (1,1022) | 1:B:81:VAL:HG11 | 1:B:81:VAL:HA    | 2        | 0.52          |
| (1,1022) | 1:B:81:VAL:HG12 | 1:B:81:VAL:HA    | 2        | 0.52          |
| (1,1022) | 1:B:81:VAL:HG13 | 1:B:81:VAL:HA    | 2        | 0.52          |
| (1,926)  | 1:B:76:SER:HB2  | 1:B:75:PHE:HD1   | 9        | 0.51          |
| (1,926)  | 1:B:76:SER:HB2  | 1:B:75:PHE:HD2   | 9        | 0.51          |
| (1,887)  | 1:B:70:LEU:HB3  | 1:B:71:GLU:H     | 2        | 0.51          |
| (1,854)  | 1:A:148:PRO:HB2 | 1:A:149:ARG:H    | 6        | 0.51          |
| (1,854)  | 1:A:148:PRO:HB3 | 1:A:149:ARG:H    | 6        | 0.51          |
| (1,848)  | 1:A:147:GLY:HA3 | 1:A:147:GLY:H    | 5        | 0.51          |
| (1,831)  | 1:A:146:ASP:HB2 | 1:A:145:VAL:HA   | 3        | 0.51          |
| (1,750)  | 1:A:136:SER:H   | 1:A:143:LEU:HD11 | 3        | 0.51          |
| (1,750)  | 1:A:136:SER:H   | 1:A:143:LEU:HD12 | 3        | 0.51          |
| (1,750)  | 1:A:136:SER:H   | 1:A:143:LEU:HD13 | 3        | 0.51          |
| (1,750)  | 1:A:136:SER:H   | 1:A:143:LEU:HD21 | 3        | 0.51          |
| (1,750)  | 1:A:136:SER:H   | 1:A:143:LEU:HD22 | 3        | 0.51          |
| (1,750)  | 1:A:136:SER:H   | 1:A:143:LEU:HD23 | 3        | 0.51          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG21 | 9        | 0.51          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG22 | 9        | 0.51          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG23 | 9        | 0.51          |
| (1,710) | 1:A:132:THR:HB   | 1:A:148:PRO:HD2  | 8        | 0.51          |
| (1,710) | 1:A:132:THR:HB   | 1:A:148:PRO:HD3  | 8        | 0.51          |
| (1,635) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 5        | 0.51          |
| (1,635) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 5        | 0.51          |
| (1,635) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 5        | 0.51          |
| (1,635) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 9        | 0.51          |
| (1,635) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 9        | 0.51          |
| (1,635) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 9        | 0.51          |
| (1,634) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 5        | 0.51          |
| (1,634) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 5        | 0.51          |
| (1,634) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 5        | 0.51          |
| (1,634) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 9        | 0.51          |
| (1,634) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 9        | 0.51          |
| (1,634) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 9        | 0.51          |
| (1,59)  | 1:A:76:SER:HB2   | 1:A:75:PHE:HD1   | 9        | 0.51          |
| (1,59)  | 1:A:76:SER:HB2   | 1:A:75:PHE:HD2   | 9        | 0.51          |
| (1,569) | 1:A:119:HIS:HA   | 1:A:101:HIS:HA   | 5        | 0.51          |
| (1,562) | 1:A:118:PHE:HA   | 1:A:118:PHE:H    | 9        | 0.51          |
| (1,553) | 1:A:118:PHE:HD1  | 1:A:103:LYS:H    | 9        | 0.51          |
| (1,553) | 1:A:118:PHE:HD2  | 1:A:103:LYS:H    | 9        | 0.51          |
| (1,540) | 1:A:116:ARG:HA   | 1:A:117:GLU:H    | 5        | 0.51          |
| (1,522) | 1:A:115:SER:HB3  | 1:A:105:GLU:HB2  | 8        | 0.51          |
| (1,522) | 1:A:115:SER:HB3  | 1:A:105:GLU:HB3  | 8        | 0.51          |
| (1,510) | 1:A:114:ILE:HG21 | 1:A:111:HIS:H    | 8        | 0.51          |
| (1,510) | 1:A:114:ILE:HG22 | 1:A:111:HIS:H    | 8        | 0.51          |
| (1,510) | 1:A:114:ILE:HG23 | 1:A:111:HIS:H    | 8        | 0.51          |
| (1,471) | 1:A:111:HIS:H    | 1:A:112:GLY:H    | 6        | 0.51          |
| (1,468) | 1:A:111:HIS:H    | 1:A:112:GLY:H    | 6        | 0.51          |
| (1,465) | 1:A:111:HIS:HB2  | 1:A:111:HIS:H    | 3        | 0.51          |
| (1,437) | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD1  | 4        | 0.51          |
| (1,437) | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD2  | 4        | 0.51          |
| (1,387) | 1:A:102:GLY:HA3  | 1:A:102:GLY:H    | 9        | 0.51          |
| (1,354) | 1:A:99:GLU:HA    | 1:A:100:VAL:H    | 6        | 0.51          |
| (1,323) | 1:A:97:VAL:HB    | 1:A:94:LEU:HB2   | 3        | 0.51          |
| (1,323) | 1:A:97:VAL:HB    | 1:A:94:LEU:HB3   | 3        | 0.51          |
| (1,323) | 1:A:97:VAL:HB    | 1:A:94:LEU:HB2   | 4        | 0.51          |
| (1,323) | 1:A:97:VAL:HB    | 1:A:94:LEU:HB3   | 4        | 0.51          |
| (1,320) | 1:A:96:ASP:HA    | 1:A:124:ILE:H    | 3        | 0.51          |
| (1,287) | 1:A:93:VAL:HA    | 1:A:98:ILE:HA    | 2        | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD2   | 3        | 0.51          |
| (1,274)  | 1:A:92:LYS:H     | 1:A:92:LYS:HD3   | 3        | 0.51          |
| (1,246)  | 1:A:89:LEU:H     | 1:A:89:LEU:HG    | 5        | 0.51          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG2   | 4        | 0.51          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG3   | 4        | 0.51          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD21  | 6        | 0.51          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD22  | 6        | 0.51          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD23  | 6        | 0.51          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD21  | 6        | 0.51          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD22  | 6        | 0.51          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD23  | 6        | 0.51          |
| (1,203)  | 1:A:84:PHE:HE1   | 1:A:116:ARG:H    | 6        | 0.51          |
| (1,203)  | 1:A:84:PHE:HE2   | 1:A:116:ARG:H    | 6        | 0.51          |
| (1,20)   | 1:A:70:LEU:HB3   | 1:A:71:GLU:H     | 2        | 0.51          |
| (1,177)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB2   | 6        | 0.51          |
| (1,1721) | 1:B:148:PRO:HB2  | 1:B:149:ARG:H    | 6        | 0.51          |
| (1,1721) | 1:B:148:PRO:HB3  | 1:B:149:ARG:H    | 6        | 0.51          |
| (1,172)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB2   | 6        | 0.51          |
| (1,1715) | 1:B:147:GLY:HA3  | 1:B:147:GLY:H    | 5        | 0.51          |
| (1,1698) | 1:B:146:ASP:HB2  | 1:B:145:VAL:HA   | 3        | 0.51          |
| (1,167)  | 1:A:81:VAL:H     | 1:A:141:GLY:HA2  | 8        | 0.51          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD11 | 3        | 0.51          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD12 | 3        | 0.51          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD13 | 3        | 0.51          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD21 | 3        | 0.51          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD22 | 3        | 0.51          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD23 | 3        | 0.51          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG21 | 9        | 0.51          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG22 | 9        | 0.51          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG23 | 9        | 0.51          |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD2  | 8        | 0.51          |
| (1,1577) | 1:B:132:THR:HB   | 1:B:148:PRO:HD3  | 8        | 0.51          |
| (1,154)  | 1:A:81:VAL:HG21  | 1:A:81:VAL:HA    | 4        | 0.51          |
| (1,154)  | 1:A:81:VAL:HG22  | 1:A:81:VAL:HA    | 4        | 0.51          |
| (1,154)  | 1:A:81:VAL:HG23  | 1:A:81:VAL:HA    | 4        | 0.51          |
| (1,1502) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 5        | 0.51          |
| (1,1502) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 5        | 0.51          |
| (1,1502) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H    | 5        | 0.51          |
| (1,1502) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 9        | 0.51          |
| (1,1502) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 9        | 0.51          |
| (1,1502) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H    | 9        | 0.51          |
| (1,1501) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 5        | 0.51          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1501) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H   | 5        | 0.51          |
| (1,1501) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H   | 5        | 0.51          |
| (1,1501) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H   | 9        | 0.51          |
| (1,1501) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H   | 9        | 0.51          |
| (1,1501) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H   | 9        | 0.51          |
| (1,1429) | 1:B:118:PHE:HA   | 1:B:118:PHE:H   | 9        | 0.51          |
| (1,1420) | 1:B:118:PHE:HD1  | 1:B:103:LYS:H   | 9        | 0.51          |
| (1,1420) | 1:B:118:PHE:HD2  | 1:B:103:LYS:H   | 9        | 0.51          |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB2 | 8        | 0.51          |
| (1,1389) | 1:B:115:SER:HB3  | 1:B:105:GLU:HB3 | 8        | 0.51          |
| (1,1377) | 1:B:114:ILE:HG21 | 1:B:111:HIS:H   | 8        | 0.51          |
| (1,1377) | 1:B:114:ILE:HG22 | 1:B:111:HIS:H   | 8        | 0.51          |
| (1,1377) | 1:B:114:ILE:HG23 | 1:B:111:HIS:H   | 8        | 0.51          |
| (1,1338) | 1:B:111:HIS:H    | 1:B:112:GLY:H   | 6        | 0.51          |
| (1,1335) | 1:B:111:HIS:H    | 1:B:112:GLY:H   | 6        | 0.51          |
| (1,1332) | 1:B:111:HIS:HB2  | 1:B:111:HIS:H   | 3        | 0.51          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD1 | 4        | 0.51          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD2 | 4        | 0.51          |
| (1,1254) | 1:B:102:GLY:HA3  | 1:B:102:GLY:H   | 9        | 0.51          |
| (1,1221) | 1:B:99:GLU:HA    | 1:B:100:VAL:H   | 6        | 0.51          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB2  | 3        | 0.51          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB3  | 3        | 0.51          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB2  | 4        | 0.51          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB3  | 4        | 0.51          |
| (1,1187) | 1:B:96:ASP:HA    | 1:B:124:ILE:H   | 3        | 0.51          |
| (1,1154) | 1:B:93:VAL:HA    | 1:B:98:ILE:HA   | 2        | 0.51          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD2  | 3        | 0.51          |
| (1,1141) | 1:B:92:LYS:H     | 1:B:92:LYS:HD3  | 3        | 0.51          |
| (1,1113) | 1:B:89:LEU:H     | 1:B:89:LEU:HG   | 5        | 0.51          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG2  | 2        | 0.51          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG3  | 2        | 0.51          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG2  | 4        | 0.51          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG3  | 4        | 0.51          |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD21 | 6        | 0.51          |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD22 | 6        | 0.51          |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD23 | 6        | 0.51          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD21 | 6        | 0.51          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD22 | 6        | 0.51          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD23 | 6        | 0.51          |
| (1,1070) | 1:B:84:PHE:HE1   | 1:B:116:ARG:H   | 6        | 0.51          |
| (1,1070) | 1:B:84:PHE:HE2   | 1:B:116:ARG:H   | 6        | 0.51          |
| (1,1044) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB2  | 6        | 0.51          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1043) | 1:B:83:HIS:HB3   | 1:B:83:HIS:HD2  | 3        | 0.51          |
| (1,1039) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB2  | 6        | 0.51          |
| (1,1034) | 1:B:81:VAL:H     | 1:B:141:GLY:HA2 | 8        | 0.51          |
| (1,974)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HG   | 4        | 0.5           |
| (1,974)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HG   | 4        | 0.5           |
| (1,974)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HG   | 4        | 0.5           |
| (1,974)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HG   | 8        | 0.5           |
| (1,974)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HG   | 8        | 0.5           |
| (1,974)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HG   | 8        | 0.5           |
| (1,974)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HG   | 9        | 0.5           |
| (1,974)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HG   | 9        | 0.5           |
| (1,974)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HG   | 9        | 0.5           |
| (1,972)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HG   | 7        | 0.5           |
| (1,972)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HG   | 7        | 0.5           |
| (1,972)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HG   | 7        | 0.5           |
| (1,855)  | 1:A:149:ARG:HB2  | 1:A:149:ARG:H   | 9        | 0.5           |
| (1,855)  | 1:A:149:ARG:HB3  | 1:A:149:ARG:H   | 9        | 0.5           |
| (1,633)  | 1:A:124:ILE:HA   | 1:A:124:ILE:H   | 5        | 0.5           |
| (1,568)  | 1:A:119:HIS:HB3  | 1:A:101:HIS:HA  | 6        | 0.5           |
| (1,566)  | 1:A:118:PHE:HA   | 1:A:119:HIS:H   | 4        | 0.5           |
| (1,566)  | 1:A:118:PHE:HA   | 1:A:119:HIS:H   | 8        | 0.5           |
| (1,565)  | 1:A:118:PHE:HB2  | 1:A:119:HIS:H   | 5        | 0.5           |
| (1,530)  | 1:A:115:SER:HB2  | 1:A:115:SER:HB3 | 4        | 0.5           |
| (1,530)  | 1:A:115:SER:HB2  | 1:A:115:SER:HB3 | 6        | 0.5           |
| (1,530)  | 1:A:115:SER:HB2  | 1:A:115:SER:HB3 | 8        | 0.5           |
| (1,518)  | 1:A:114:ILE:HG21 | 1:A:114:ILE:H   | 8        | 0.5           |
| (1,518)  | 1:A:114:ILE:HG22 | 1:A:114:ILE:H   | 8        | 0.5           |
| (1,518)  | 1:A:114:ILE:HG23 | 1:A:114:ILE:H   | 8        | 0.5           |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB2 | 4        | 0.5           |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB3 | 4        | 0.5           |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB2 | 4        | 0.5           |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB3 | 4        | 0.5           |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB2 | 4        | 0.5           |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB3 | 4        | 0.5           |
| (1,488)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB2 | 7        | 0.5           |
| (1,300)  | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB2  | 5        | 0.5           |
| (1,300)  | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB3  | 5        | 0.5           |
| (1,271)  | 1:A:91:VAL:HB    | 1:A:92:LYS:H    | 7        | 0.5           |
| (1,254)  | 1:A:89:LEU:HD11  | 1:A:91:VAL:HB   | 6        | 0.5           |
| (1,254)  | 1:A:89:LEU:HD12  | 1:A:91:VAL:HB   | 6        | 0.5           |
| (1,254)  | 1:A:89:LEU:HD13  | 1:A:91:VAL:HB   | 6        | 0.5           |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG2  | 3        | 0.5           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG3  | 3        | 0.5           |
| (1,215)  | 1:A:85:SER:HB3   | 1:A:89:LEU:H    | 1        | 0.5           |
| (1,198)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H    | 9        | 0.5           |
| (1,198)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H    | 9        | 0.5           |
| (1,196)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H    | 9        | 0.5           |
| (1,196)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H    | 9        | 0.5           |
| (1,1580) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HB2 | 2        | 0.5           |
| (1,1580) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HB3 | 2        | 0.5           |
| (1,1580) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HB2 | 2        | 0.5           |
| (1,1580) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HB3 | 2        | 0.5           |
| (1,1580) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HB2 | 2        | 0.5           |
| (1,1580) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HB3 | 2        | 0.5           |
| (1,1500) | 1:B:124:ILE:HA   | 1:B:124:ILE:H   | 5        | 0.5           |
| (1,1435) | 1:B:119:HIS:HB3  | 1:B:101:HIS:HA  | 6        | 0.5           |
| (1,1433) | 1:B:118:PHE:HA   | 1:B:119:HIS:H   | 4        | 0.5           |
| (1,1433) | 1:B:118:PHE:HA   | 1:B:119:HIS:H   | 8        | 0.5           |
| (1,1432) | 1:B:118:PHE:HB2  | 1:B:119:HIS:H   | 5        | 0.5           |
| (1,1397) | 1:B:115:SER:HB2  | 1:B:115:SER:HB3 | 4        | 0.5           |
| (1,1397) | 1:B:115:SER:HB2  | 1:B:115:SER:HB3 | 8        | 0.5           |
| (1,1385) | 1:B:114:ILE:HG21 | 1:B:114:ILE:H   | 8        | 0.5           |
| (1,1385) | 1:B:114:ILE:HG22 | 1:B:114:ILE:H   | 8        | 0.5           |
| (1,1385) | 1:B:114:ILE:HG23 | 1:B:114:ILE:H   | 8        | 0.5           |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB2 | 4        | 0.5           |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB3 | 4        | 0.5           |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB2 | 4        | 0.5           |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB3 | 4        | 0.5           |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB2 | 4        | 0.5           |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB3 | 4        | 0.5           |
| (1,1355) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB2 | 7        | 0.5           |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB2  | 5        | 0.5           |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB3  | 5        | 0.5           |
| (1,1138) | 1:B:91:VAL:HB    | 1:B:92:LYS:H    | 7        | 0.5           |
| (1,1121) | 1:B:89:LEU:HD11  | 1:B:91:VAL:HB   | 6        | 0.5           |
| (1,1121) | 1:B:89:LEU:HD12  | 1:B:91:VAL:HB   | 6        | 0.5           |
| (1,1121) | 1:B:89:LEU:HD13  | 1:B:91:VAL:HB   | 6        | 0.5           |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG2  | 3        | 0.5           |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG3  | 3        | 0.5           |
| (1,1082) | 1:B:85:SER:HB3   | 1:B:89:LEU:H    | 1        | 0.5           |
| (1,107)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:HG   | 4        | 0.5           |
| (1,107)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:HG   | 4        | 0.5           |
| (1,107)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:HG   | 4        | 0.5           |
| (1,107)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:HG   | 9        | 0.5           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,107)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:HG   | 9        | 0.5           |
| (1,107)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:HG   | 9        | 0.5           |
| (1,1065) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H    | 9        | 0.5           |
| (1,1065) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H    | 9        | 0.5           |
| (1,1063) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H    | 9        | 0.5           |
| (1,1063) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H    | 9        | 0.5           |
| (1,105)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HG   | 7        | 0.5           |
| (1,105)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HG   | 7        | 0.5           |
| (1,105)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HG   | 7        | 0.5           |
| (1,950)  | 1:B:77:VAL:HG11  | 1:B:68:MET:HA   | 5        | 0.49          |
| (1,950)  | 1:B:77:VAL:HG12  | 1:B:68:MET:HA   | 5        | 0.49          |
| (1,950)  | 1:B:77:VAL:HG13  | 1:B:68:MET:HA   | 5        | 0.49          |
| (1,83)   | 1:A:77:VAL:HG11  | 1:A:68:MET:HA   | 5        | 0.49          |
| (1,83)   | 1:A:77:VAL:HG12  | 1:A:68:MET:HA   | 5        | 0.49          |
| (1,83)   | 1:A:77:VAL:HG13  | 1:A:68:MET:HA   | 5        | 0.49          |
| (1,717)  | 1:A:133:ILE:HG21 | 1:A:132:THR:H   | 3        | 0.49          |
| (1,717)  | 1:A:133:ILE:HG22 | 1:A:132:THR:H   | 3        | 0.49          |
| (1,717)  | 1:A:133:ILE:HG23 | 1:A:132:THR:H   | 3        | 0.49          |
| (1,686)  | 1:A:129:ASP:H    | 1:A:132:THR:HG1 | 7        | 0.49          |
| (1,586)  | 1:A:121:LYS:HA   | 1:A:122:TYR:H   | 2        | 0.49          |
| (1,562)  | 1:A:118:PHE:HA   | 1:A:118:PHE:H   | 1        | 0.49          |
| (1,530)  | 1:A:115:SER:HB2  | 1:A:115:SER:HB3 | 2        | 0.49          |
| (1,530)  | 1:A:115:SER:HB2  | 1:A:115:SER:HB3 | 5        | 0.49          |
| (1,530)  | 1:A:115:SER:HB2  | 1:A:115:SER:HB3 | 7        | 0.49          |
| (1,524)  | 1:A:115:SER:HB2  | 1:A:106:GLU:H   | 9        | 0.49          |
| (1,469)  | 1:A:111:HIS:HB2  | 1:A:112:GLY:H   | 3        | 0.49          |
| (1,376)  | 1:A:101:HIS:HB2  | 1:A:101:HIS:HD2 | 1        | 0.49          |
| (1,354)  | 1:A:99:GLU:HA    | 1:A:100:VAL:H   | 2        | 0.49          |
| (1,323)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HB2  | 9        | 0.49          |
| (1,323)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HB3  | 9        | 0.49          |
| (1,239)  | 1:A:89:LEU:H     | 1:A:87:GLU:HA   | 5        | 0.49          |
| (1,218)  | 1:A:86:PRO:HB2   | 1:A:85:SER:HA   | 1        | 0.49          |
| (1,218)  | 1:A:86:PRO:HB3   | 1:A:85:SER:HA   | 1        | 0.49          |
| (1,195)  | 1:A:84:PHE:HD1   | 1:A:84:PHE:H    | 2        | 0.49          |
| (1,195)  | 1:A:84:PHE:HD2   | 1:A:84:PHE:H    | 2        | 0.49          |
| (1,184)  | 1:A:83:HIS:H     | 1:A:84:PHE:H    | 7        | 0.49          |
| (1,183)  | 1:A:83:HIS:H     | 1:A:84:PHE:H    | 7        | 0.49          |
| (1,1736) | 1:A:111:HIS:HB2  | 1:B:122:TYR:HE1 | 3        | 0.49          |
| (1,1736) | 1:A:111:HIS:HB2  | 1:B:122:TYR:HE2 | 3        | 0.49          |
| (1,1722) | 1:B:149:ARG:HB2  | 1:B:149:ARG:H   | 9        | 0.49          |
| (1,1722) | 1:B:149:ARG:HB3  | 1:B:149:ARG:H   | 9        | 0.49          |
| (1,1584) | 1:B:133:ILE:HG21 | 1:B:132:THR:H   | 3        | 0.49          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1584) | 1:B:133:ILE:HG22 | 1:B:132:THR:H   | 3        | 0.49          |
| (1,1584) | 1:B:133:ILE:HG23 | 1:B:132:THR:H   | 3        | 0.49          |
| (1,1566) | 1:B:132:THR:HG1  | 1:B:132:THR:H   | 4        | 0.49          |
| (1,154)  | 1:A:81:VAL:HG21  | 1:A:81:VAL:HA   | 1        | 0.49          |
| (1,154)  | 1:A:81:VAL:HG22  | 1:A:81:VAL:HA   | 1        | 0.49          |
| (1,154)  | 1:A:81:VAL:HG23  | 1:A:81:VAL:HA   | 1        | 0.49          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG21 | 4        | 0.49          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG22 | 4        | 0.49          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG23 | 4        | 0.49          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG21 | 4        | 0.49          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG22 | 4        | 0.49          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG23 | 4        | 0.49          |
| (1,1453) | 1:B:121:LYS:HA   | 1:B:122:TYR:H   | 2        | 0.49          |
| (1,1429) | 1:B:118:PHE:HA   | 1:B:118:PHE:H   | 1        | 0.49          |
| (1,1397) | 1:B:115:SER:HB2  | 1:B:115:SER:HB3 | 2        | 0.49          |
| (1,1397) | 1:B:115:SER:HB2  | 1:B:115:SER:HB3 | 5        | 0.49          |
| (1,1397) | 1:B:115:SER:HB2  | 1:B:115:SER:HB3 | 6        | 0.49          |
| (1,1397) | 1:B:115:SER:HB2  | 1:B:115:SER:HB3 | 7        | 0.49          |
| (1,1391) | 1:B:115:SER:HB2  | 1:B:106:GLU:H   | 9        | 0.49          |
| (1,1336) | 1:B:111:HIS:HB2  | 1:B:112:GLY:H   | 3        | 0.49          |
| (1,1243) | 1:B:101:HIS:HB2  | 1:B:101:HIS:HD2 | 1        | 0.49          |
| (1,1221) | 1:B:99:GLU:HA    | 1:B:100:VAL:H   | 2        | 0.49          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB2  | 9        | 0.49          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB3  | 9        | 0.49          |
| (1,112)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HD1 | 8        | 0.49          |
| (1,112)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HD2 | 8        | 0.49          |
| (1,112)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HD1 | 8        | 0.49          |
| (1,112)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HD2 | 8        | 0.49          |
| (1,112)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HD1 | 8        | 0.49          |
| (1,112)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HD2 | 8        | 0.49          |
| (1,1106) | 1:B:89:LEU:H     | 1:B:87:GLU:HA   | 5        | 0.49          |
| (1,1085) | 1:B:86:PRO:HB2   | 1:B:85:SER:HA   | 1        | 0.49          |
| (1,1085) | 1:B:86:PRO:HB3   | 1:B:85:SER:HA   | 1        | 0.49          |
| (1,107)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:HG   | 8        | 0.49          |
| (1,107)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:HG   | 8        | 0.49          |
| (1,107)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:HG   | 8        | 0.49          |
| (1,1062) | 1:B:84:PHE:HD1   | 1:B:84:PHE:H    | 2        | 0.49          |
| (1,1062) | 1:B:84:PHE:HD2   | 1:B:84:PHE:H    | 2        | 0.49          |
| (1,1051) | 1:B:83:HIS:H     | 1:B:84:PHE:H    | 7        | 0.49          |
| (1,1050) | 1:B:83:HIS:H     | 1:B:84:PHE:H    | 7        | 0.49          |
| (1,1021) | 1:B:81:VAL:HG21  | 1:B:81:VAL:HA   | 1        | 0.49          |
| (1,1021) | 1:B:81:VAL:HG22  | 1:B:81:VAL:HA   | 1        | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1021) | 1:B:81:VAL:HG23  | 1:B:81:VAL:HA    | 1        | 0.49          |
| (1,1021) | 1:B:81:VAL:HG21  | 1:B:81:VAL:HA    | 4        | 0.49          |
| (1,1021) | 1:B:81:VAL:HG22  | 1:B:81:VAL:HA    | 4        | 0.49          |
| (1,1021) | 1:B:81:VAL:HG23  | 1:B:81:VAL:HA    | 4        | 0.49          |
| (1,979)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HD1  | 8        | 0.48          |
| (1,979)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HD2  | 8        | 0.48          |
| (1,979)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HD1  | 8        | 0.48          |
| (1,979)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HD2  | 8        | 0.48          |
| (1,979)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HD1  | 8        | 0.48          |
| (1,979)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HD2  | 8        | 0.48          |
| (1,948)  | 1:B:77:VAL:HG11  | 1:B:68:MET:HE1   | 8        | 0.48          |
| (1,948)  | 1:B:77:VAL:HG11  | 1:B:68:MET:HE2   | 8        | 0.48          |
| (1,948)  | 1:B:77:VAL:HG11  | 1:B:68:MET:HE3   | 8        | 0.48          |
| (1,948)  | 1:B:77:VAL:HG12  | 1:B:68:MET:HE1   | 8        | 0.48          |
| (1,948)  | 1:B:77:VAL:HG12  | 1:B:68:MET:HE2   | 8        | 0.48          |
| (1,948)  | 1:B:77:VAL:HG12  | 1:B:68:MET:HE3   | 8        | 0.48          |
| (1,948)  | 1:B:77:VAL:HG13  | 1:B:68:MET:HE1   | 8        | 0.48          |
| (1,948)  | 1:B:77:VAL:HG13  | 1:B:68:MET:HE2   | 8        | 0.48          |
| (1,948)  | 1:B:77:VAL:HG13  | 1:B:68:MET:HE3   | 8        | 0.48          |
| (1,875)  | 1:B:68:MET:HG2   | 1:B:68:MET:H     | 9        | 0.48          |
| (1,875)  | 1:B:68:MET:HG3   | 1:B:68:MET:H     | 9        | 0.48          |
| (1,819)  | 1:A:145:VAL:HG21 | 1:A:145:VAL:H    | 8        | 0.48          |
| (1,819)  | 1:A:145:VAL:HG22 | 1:A:145:VAL:H    | 8        | 0.48          |
| (1,819)  | 1:A:145:VAL:HG23 | 1:A:145:VAL:H    | 8        | 0.48          |
| (1,81)   | 1:A:77:VAL:HG11  | 1:A:68:MET:HE1   | 8        | 0.48          |
| (1,81)   | 1:A:77:VAL:HG11  | 1:A:68:MET:HE2   | 8        | 0.48          |
| (1,81)   | 1:A:77:VAL:HG11  | 1:A:68:MET:HE3   | 8        | 0.48          |
| (1,81)   | 1:A:77:VAL:HG12  | 1:A:68:MET:HE1   | 8        | 0.48          |
| (1,81)   | 1:A:77:VAL:HG12  | 1:A:68:MET:HE2   | 8        | 0.48          |
| (1,81)   | 1:A:77:VAL:HG12  | 1:A:68:MET:HE3   | 8        | 0.48          |
| (1,81)   | 1:A:77:VAL:HG13  | 1:A:68:MET:HE1   | 8        | 0.48          |
| (1,81)   | 1:A:77:VAL:HG13  | 1:A:68:MET:HE2   | 8        | 0.48          |
| (1,81)   | 1:A:77:VAL:HG13  | 1:A:68:MET:HE3   | 8        | 0.48          |
| (1,8)    | 1:A:68:MET:HG2   | 1:A:68:MET:H     | 9        | 0.48          |
| (1,8)    | 1:A:68:MET:HG3   | 1:A:68:MET:H     | 9        | 0.48          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD11 | 1        | 0.48          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD12 | 1        | 0.48          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD13 | 1        | 0.48          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD21 | 1        | 0.48          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD22 | 1        | 0.48          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD23 | 1        | 0.48          |
| (1,569)  | 1:A:119:HIS:HA   | 1:A:101:HIS:HA   | 4        | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,544)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 2        | 0.48          |
| (1,543)  | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 2        | 0.48          |
| (1,540)  | 1:A:116:ARG:HA   | 1:A:117:GLU:H    | 1        | 0.48          |
| (1,530)  | 1:A:115:SER:HB2  | 1:A:115:SER:HB3  | 1        | 0.48          |
| (1,530)  | 1:A:115:SER:HB2  | 1:A:115:SER:HB3  | 3        | 0.48          |
| (1,523)  | 1:A:115:SER:HB3  | 1:A:106:GLU:H    | 1        | 0.48          |
| (1,492)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HE1  | 7        | 0.48          |
| (1,492)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HE2  | 7        | 0.48          |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG2   | 8        | 0.48          |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG3   | 8        | 0.48          |
| (1,354)  | 1:A:99:GLU:HA    | 1:A:100:VAL:H    | 1        | 0.48          |
| (1,244)  | 1:A:89:LEU:HD21  | 1:A:88:GLU:H     | 8        | 0.48          |
| (1,244)  | 1:A:89:LEU:HD22  | 1:A:88:GLU:H     | 8        | 0.48          |
| (1,244)  | 1:A:89:LEU:HD23  | 1:A:88:GLU:H     | 8        | 0.48          |
| (1,243)  | 1:A:89:LEU:HD11  | 1:A:88:GLU:H     | 9        | 0.48          |
| (1,243)  | 1:A:89:LEU:HD12  | 1:A:88:GLU:H     | 9        | 0.48          |
| (1,243)  | 1:A:89:LEU:HD13  | 1:A:88:GLU:H     | 9        | 0.48          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG2   | 1        | 0.48          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG3   | 1        | 0.48          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG2   | 8        | 0.48          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG3   | 8        | 0.48          |
| (1,192)  | 1:A:84:PHE:HD1   | 1:A:83:HIS:HB3   | 8        | 0.48          |
| (1,192)  | 1:A:84:PHE:HD2   | 1:A:83:HIS:HB3   | 8        | 0.48          |
| (1,185)  | 1:A:83:HIS:HB3   | 1:A:104:HIS:HB2  | 8        | 0.48          |
| (1,184)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 2        | 0.48          |
| (1,183)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 2        | 0.48          |
| (1,1770) | 1:A:123:ARG:HD2  | 1:B:113:PHE:H    | 1        | 0.48          |
| (1,1770) | 1:A:123:ARG:HD3  | 1:B:113:PHE:H    | 1        | 0.48          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD11 | 1        | 0.48          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD12 | 1        | 0.48          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD13 | 1        | 0.48          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD21 | 1        | 0.48          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD22 | 1        | 0.48          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD23 | 1        | 0.48          |
| (1,157)  | 1:A:81:VAL:HG21  | 1:A:81:VAL:H     | 5        | 0.48          |
| (1,157)  | 1:A:81:VAL:HG22  | 1:A:81:VAL:H     | 5        | 0.48          |
| (1,157)  | 1:A:81:VAL:HG23  | 1:A:81:VAL:H     | 5        | 0.48          |
| (1,1502) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 3        | 0.48          |
| (1,1502) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 3        | 0.48          |
| (1,1502) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H    | 3        | 0.48          |
| (1,1501) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 3        | 0.48          |
| (1,1501) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 3        | 0.48          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1501) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H   | 3        | 0.48          |
| (1,1436) | 1:B:119:HIS:HA   | 1:B:101:HIS:HA  | 4        | 0.48          |
| (1,1411) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA  | 2        | 0.48          |
| (1,1410) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA  | 2        | 0.48          |
| (1,1407) | 1:B:116:ARG:HA   | 1:B:117:GLU:H   | 1        | 0.48          |
| (1,1397) | 1:B:115:SER:HB2  | 1:B:115:SER:HB3 | 1        | 0.48          |
| (1,1397) | 1:B:115:SER:HB2  | 1:B:115:SER:HB3 | 3        | 0.48          |
| (1,1397) | 1:B:115:SER:HB2  | 1:B:115:SER:HB3 | 9        | 0.48          |
| (1,1390) | 1:B:115:SER:HB3  | 1:B:106:GLU:H   | 1        | 0.48          |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE1 | 7        | 0.48          |
| (1,1359) | 1:B:113:PHE:HA   | 1:B:113:PHE:HE2 | 7        | 0.48          |
| (1,1332) | 1:B:111:HIS:HB2  | 1:B:111:HIS:H   | 8        | 0.48          |
| (1,1262) | 1:B:103:LYS:HG2  | 1:B:103:LYS:H   | 4        | 0.48          |
| (1,1262) | 1:B:103:LYS:HG3  | 1:B:103:LYS:H   | 4        | 0.48          |
| (1,1260) | 1:B:103:LYS:H    | 1:B:88:GLU:HG2  | 8        | 0.48          |
| (1,1260) | 1:B:103:LYS:H    | 1:B:88:GLU:HG3  | 8        | 0.48          |
| (1,1243) | 1:B:101:HIS:HB2  | 1:B:101:HIS:HD2 | 7        | 0.48          |
| (1,1221) | 1:B:99:GLU:HA    | 1:B:100:VAL:H   | 1        | 0.48          |
| (1,1111) | 1:B:89:LEU:HD21  | 1:B:88:GLU:H    | 8        | 0.48          |
| (1,1111) | 1:B:89:LEU:HD22  | 1:B:88:GLU:H    | 8        | 0.48          |
| (1,1111) | 1:B:89:LEU:HD23  | 1:B:88:GLU:H    | 8        | 0.48          |
| (1,1110) | 1:B:89:LEU:HD11  | 1:B:88:GLU:H    | 9        | 0.48          |
| (1,1110) | 1:B:89:LEU:HD12  | 1:B:88:GLU:H    | 9        | 0.48          |
| (1,1110) | 1:B:89:LEU:HD13  | 1:B:88:GLU:H    | 9        | 0.48          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG2  | 1        | 0.48          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG3  | 1        | 0.48          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG2  | 8        | 0.48          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG3  | 8        | 0.48          |
| (1,1059) | 1:B:84:PHE:HD1   | 1:B:83:HIS:HB3  | 8        | 0.48          |
| (1,1059) | 1:B:84:PHE:HD2   | 1:B:83:HIS:HB3  | 8        | 0.48          |
| (1,1052) | 1:B:83:HIS:HB3   | 1:B:104:HIS:HB2 | 8        | 0.48          |
| (1,1051) | 1:B:83:HIS:H     | 1:B:84:PHE:H    | 2        | 0.48          |
| (1,1050) | 1:B:83:HIS:H     | 1:B:84:PHE:H    | 2        | 0.48          |
| (1,1024) | 1:B:81:VAL:HG21  | 1:B:81:VAL:H    | 5        | 0.48          |
| (1,1024) | 1:B:81:VAL:HG22  | 1:B:81:VAL:H    | 5        | 0.48          |
| (1,1024) | 1:B:81:VAL:HG23  | 1:B:81:VAL:H    | 5        | 0.48          |
| (1,787)  | 1:A:143:LEU:H    | 1:A:79:LEU:H    | 6        | 0.47          |
| (1,715)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HG2 | 3        | 0.47          |
| (1,715)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HG3 | 3        | 0.47          |
| (1,715)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HG2 | 3        | 0.47          |
| (1,715)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HG3 | 3        | 0.47          |
| (1,715)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HG2 | 3        | 0.47          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,715) | 1:A:133:ILE:HD13 | 1:A:130:PRO:HG3 | 3        | 0.47          |
| (1,700) | 1:A:132:THR:HG21 | 1:A:132:THR:H   | 1        | 0.47          |
| (1,700) | 1:A:132:THR:HG22 | 1:A:132:THR:H   | 1        | 0.47          |
| (1,700) | 1:A:132:THR:HG23 | 1:A:132:THR:H   | 1        | 0.47          |
| (1,635) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H   | 7        | 0.47          |
| (1,635) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H   | 7        | 0.47          |
| (1,635) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H   | 7        | 0.47          |
| (1,634) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H   | 7        | 0.47          |
| (1,634) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H   | 7        | 0.47          |
| (1,634) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H   | 7        | 0.47          |
| (1,633) | 1:A:124:ILE:HA   | 1:A:124:ILE:H   | 8        | 0.47          |
| (1,589) | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG21 | 4        | 0.47          |
| (1,589) | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG22 | 4        | 0.47          |
| (1,589) | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG23 | 4        | 0.47          |
| (1,589) | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG21 | 4        | 0.47          |
| (1,589) | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG22 | 4        | 0.47          |
| (1,589) | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG23 | 4        | 0.47          |
| (1,579) | 1:A:119:HIS:H    | 1:A:120:ARG:H   | 1        | 0.47          |
| (1,562) | 1:A:118:PHE:HA   | 1:A:118:PHE:H   | 2        | 0.47          |
| (1,562) | 1:A:118:PHE:HA   | 1:A:118:PHE:H   | 7        | 0.47          |
| (1,530) | 1:A:115:SER:HB2  | 1:A:115:SER:HB3 | 9        | 0.47          |
| (1,488) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB2 | 5        | 0.47          |
| (1,468) | 1:A:111:HIS:H    | 1:A:112:GLY:H   | 8        | 0.47          |
| (1,465) | 1:A:111:HIS:HB2  | 1:A:111:HIS:H   | 8        | 0.47          |
| (1,464) | 1:A:111:HIS:H    | 1:A:111:HIS:HD2 | 2        | 0.47          |
| (1,407) | 1:A:104:HIS:HA   | 1:A:105:GLU:H   | 2        | 0.47          |
| (1,407) | 1:A:104:HIS:HA   | 1:A:105:GLU:H   | 4        | 0.47          |
| (1,395) | 1:A:103:LYS:HG2  | 1:A:103:LYS:H   | 4        | 0.47          |
| (1,395) | 1:A:103:LYS:HG3  | 1:A:103:LYS:H   | 4        | 0.47          |
| (1,365) | 1:A:100:VAL:HG11 | 1:A:102:GLY:H   | 9        | 0.47          |
| (1,365) | 1:A:100:VAL:HG12 | 1:A:102:GLY:H   | 9        | 0.47          |
| (1,365) | 1:A:100:VAL:HG13 | 1:A:102:GLY:H   | 9        | 0.47          |
| (1,330) | 1:A:97:VAL:HA    | 1:A:123:ARG:HA  | 3        | 0.47          |
| (1,329) | 1:A:97:VAL:HA    | 1:A:123:ARG:HA  | 3        | 0.47          |
| (1,301) | 1:A:95:GLY:H     | 1:A:94:LEU:HG   | 5        | 0.47          |
| (1,285) | 1:A:93:VAL:HG11  | 1:A:93:VAL:H    | 5        | 0.47          |
| (1,285) | 1:A:93:VAL:HG12  | 1:A:93:VAL:H    | 5        | 0.47          |
| (1,285) | 1:A:93:VAL:HG13  | 1:A:93:VAL:H    | 5        | 0.47          |
| (1,285) | 1:A:93:VAL:HG21  | 1:A:93:VAL:H    | 5        | 0.47          |
| (1,285) | 1:A:93:VAL:HG22  | 1:A:93:VAL:H    | 5        | 0.47          |
| (1,285) | 1:A:93:VAL:HG23  | 1:A:93:VAL:H    | 5        | 0.47          |
| (1,281) | 1:A:92:LYS:H     | 1:A:101:HIS:H   | 5        | 0.47          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,280)  | 1:A:92:LYS:H     | 1:A:100:VAL:HA  | 5        | 0.47          |
| (1,179)  | 1:A:83:HIS:HA    | 1:A:83:HIS:H    | 4        | 0.47          |
| (1,177)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB2  | 8        | 0.47          |
| (1,172)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB2  | 8        | 0.47          |
| (1,171)  | 1:A:83:HIS:H     | 1:A:82:LYS:HG2  | 9        | 0.47          |
| (1,171)  | 1:A:83:HIS:H     | 1:A:82:LYS:HG3  | 9        | 0.47          |
| (1,1686) | 1:B:145:VAL:HG21 | 1:B:145:VAL:H   | 8        | 0.47          |
| (1,1686) | 1:B:145:VAL:HG22 | 1:B:145:VAL:H   | 8        | 0.47          |
| (1,1686) | 1:B:145:VAL:HG23 | 1:B:145:VAL:H   | 8        | 0.47          |
| (1,1654) | 1:B:143:LEU:H    | 1:B:79:LEU:H    | 6        | 0.47          |
| (1,159)  | 1:A:81:VAL:H     | 1:A:82:LYS:H    | 4        | 0.47          |
| (1,1582) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HG2 | 3        | 0.47          |
| (1,1582) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HG3 | 3        | 0.47          |
| (1,1582) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HG2 | 3        | 0.47          |
| (1,1582) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HG3 | 3        | 0.47          |
| (1,1582) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HG2 | 3        | 0.47          |
| (1,1582) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HG3 | 3        | 0.47          |
| (1,1567) | 1:B:132:THR:HG21 | 1:B:132:THR:H   | 1        | 0.47          |
| (1,1567) | 1:B:132:THR:HG22 | 1:B:132:THR:H   | 1        | 0.47          |
| (1,1567) | 1:B:132:THR:HG23 | 1:B:132:THR:H   | 1        | 0.47          |
| (1,1502) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H   | 7        | 0.47          |
| (1,1502) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H   | 7        | 0.47          |
| (1,1502) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H   | 7        | 0.47          |
| (1,1501) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H   | 7        | 0.47          |
| (1,1501) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H   | 7        | 0.47          |
| (1,1501) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H   | 7        | 0.47          |
| (1,1500) | 1:B:124:ILE:HA   | 1:B:124:ILE:H   | 8        | 0.47          |
| (1,1446) | 1:B:119:HIS:H    | 1:B:120:ARG:H   | 1        | 0.47          |
| (1,1429) | 1:B:118:PHE:HA   | 1:B:118:PHE:H   | 2        | 0.47          |
| (1,1335) | 1:B:111:HIS:H    | 1:B:112:GLY:H   | 8        | 0.47          |
| (1,1331) | 1:B:111:HIS:H    | 1:B:111:HIS:HD2 | 2        | 0.47          |
| (1,1274) | 1:B:104:HIS:HA   | 1:B:105:GLU:H   | 2        | 0.47          |
| (1,1274) | 1:B:104:HIS:HA   | 1:B:105:GLU:H   | 4        | 0.47          |
| (1,1197) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 3        | 0.47          |
| (1,1196) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 3        | 0.47          |
| (1,1168) | 1:B:95:GLY:H     | 1:B:94:LEU:HG   | 5        | 0.47          |
| (1,1148) | 1:B:92:LYS:H     | 1:B:101:HIS:H   | 5        | 0.47          |
| (1,1147) | 1:B:92:LYS:H     | 1:B:100:VAL:HA  | 5        | 0.47          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG2  | 6        | 0.47          |
| (1,1107) | 1:B:89:LEU:H     | 1:B:88:GLU:HG3  | 6        | 0.47          |
| (1,1046) | 1:B:83:HIS:HA    | 1:B:83:HIS:H    | 4        | 0.47          |
| (1,1044) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB2  | 8        | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1039) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB2   | 8        | 0.47          |
| (1,1038) | 1:B:83:HIS:H     | 1:B:82:LYS:HG2   | 9        | 0.47          |
| (1,1038) | 1:B:83:HIS:H     | 1:B:82:LYS:HG3   | 9        | 0.47          |
| (1,1026) | 1:B:81:VAL:H     | 1:B:82:LYS:H     | 4        | 0.47          |
| (1,974)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HG    | 7        | 0.46          |
| (1,974)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HG    | 7        | 0.46          |
| (1,974)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HG    | 7        | 0.46          |
| (1,930)  | 1:B:76:SER:HB2   | 1:B:77:VAL:H     | 2        | 0.46          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD11  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD12  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD13  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD21  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD22  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD23  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD11  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD12  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD13  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD21  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD22  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD23  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD11  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD12  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD13  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD21  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD22  | 3        | 0.46          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD23  | 3        | 0.46          |
| (1,866)  | 1:A:152:VAL:H    | 1:A:151:GLN:H    | 8        | 0.46          |
| (1,843)  | 1:A:147:GLY:HA2  | 1:A:133:ILE:HB   | 3        | 0.46          |
| (1,819)  | 1:A:145:VAL:HG21 | 1:A:145:VAL:H    | 7        | 0.46          |
| (1,819)  | 1:A:145:VAL:HG22 | 1:A:145:VAL:H    | 7        | 0.46          |
| (1,819)  | 1:A:145:VAL:HG23 | 1:A:145:VAL:H    | 7        | 0.46          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD11 | 5        | 0.46          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD12 | 5        | 0.46          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD13 | 5        | 0.46          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD21 | 5        | 0.46          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD22 | 5        | 0.46          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD23 | 5        | 0.46          |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB2  | 4        | 0.46          |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB3  | 4        | 0.46          |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB2  | 8        | 0.46          |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB3  | 8        | 0.46          |
| (1,635)  | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 3        | 0.46          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,635) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 3        | 0.46          |
| (1,635) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 3        | 0.46          |
| (1,634) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 3        | 0.46          |
| (1,634) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 3        | 0.46          |
| (1,634) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 3        | 0.46          |
| (1,633) | 1:A:124:ILE:HA   | 1:A:124:ILE:H    | 3        | 0.46          |
| (1,63)  | 1:A:76:SER:HB2   | 1:A:77:VAL:H     | 2        | 0.46          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG12 | 4        | 0.46          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG13 | 4        | 0.46          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG12 | 4        | 0.46          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG13 | 4        | 0.46          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG12 | 4        | 0.46          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG13 | 4        | 0.46          |
| (1,586) | 1:A:121:LYS:HA   | 1:A:122:TYR:H    | 6        | 0.46          |
| (1,571) | 1:A:119:HIS:HA   | 1:A:101:HIS:HD2  | 3        | 0.46          |
| (1,509) | 1:A:114:ILE:HG21 | 1:A:109:ASP:H    | 3        | 0.46          |
| (1,509) | 1:A:114:ILE:HG22 | 1:A:109:ASP:H    | 3        | 0.46          |
| (1,509) | 1:A:114:ILE:HG23 | 1:A:109:ASP:H    | 3        | 0.46          |
| (1,491) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 5        | 0.46          |
| (1,489) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 5        | 0.46          |
| (1,488) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB2  | 2        | 0.46          |
| (1,488) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB2  | 6        | 0.46          |
| (1,430) | 1:A:107:ARG:H    | 1:A:108:GLN:H    | 9        | 0.46          |
| (1,407) | 1:A:104:HIS:HA   | 1:A:105:GLU:H    | 1        | 0.46          |
| (1,376) | 1:A:101:HIS:HB2  | 1:A:101:HIS:HD2  | 4        | 0.46          |
| (1,346) | 1:A:98:ILE:H     | 1:A:122:TYR:H    | 7        | 0.46          |
| (1,345) | 1:A:98:ILE:H     | 1:A:122:TYR:H    | 7        | 0.46          |
| (1,337) | 1:A:98:ILE:HD11  | 1:A:98:ILE:HB    | 8        | 0.46          |
| (1,337) | 1:A:98:ILE:HD12  | 1:A:98:ILE:HB    | 8        | 0.46          |
| (1,337) | 1:A:98:ILE:HD13  | 1:A:98:ILE:HB    | 8        | 0.46          |
| (1,323) | 1:A:97:VAL:HB    | 1:A:94:LEU:HB2   | 5        | 0.46          |
| (1,323) | 1:A:97:VAL:HB    | 1:A:94:LEU:HB3   | 5        | 0.46          |
| (1,300) | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB2   | 6        | 0.46          |
| (1,300) | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB3   | 6        | 0.46          |
| (1,297) | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD11  | 5        | 0.46          |
| (1,297) | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD12  | 5        | 0.46          |
| (1,297) | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD13  | 5        | 0.46          |
| (1,297) | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD21  | 5        | 0.46          |
| (1,297) | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD22  | 5        | 0.46          |
| (1,297) | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD23  | 5        | 0.46          |
| (1,287) | 1:A:93:VAL:HA    | 1:A:98:ILE:HA    | 8        | 0.46          |
| (1,287) | 1:A:93:VAL:HA    | 1:A:98:ILE:HA    | 9        | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,259)  | 1:A:89:LEU:HD11  | 1:A:103:LYS:H    | 9        | 0.46          |
| (1,259)  | 1:A:89:LEU:HD12  | 1:A:103:LYS:H    | 9        | 0.46          |
| (1,259)  | 1:A:89:LEU:HD13  | 1:A:103:LYS:H    | 9        | 0.46          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG2   | 6        | 0.46          |
| (1,240)  | 1:A:89:LEU:H     | 1:A:88:GLU:HG3   | 6        | 0.46          |
| (1,184)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 3        | 0.46          |
| (1,183)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 3        | 0.46          |
| (1,179)  | 1:A:83:HIS:HA    | 1:A:83:HIS:H     | 2        | 0.46          |
| (1,1756) | 1:A:118:PHE:HA   | 1:B:117:GLU:H    | 9        | 0.46          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE1  | 9        | 0.46          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE2  | 9        | 0.46          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE1  | 9        | 0.46          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE2  | 9        | 0.46          |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE1  | 9        | 0.46          |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE2  | 9        | 0.46          |
| (1,1733) | 1:B:152:VAL:H    | 1:B:151:GLN:H    | 8        | 0.46          |
| (1,1710) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HB   | 3        | 0.46          |
| (1,1686) | 1:B:145:VAL:HG21 | 1:B:145:VAL:H    | 7        | 0.46          |
| (1,1686) | 1:B:145:VAL:HG22 | 1:B:145:VAL:H    | 7        | 0.46          |
| (1,1686) | 1:B:145:VAL:HG23 | 1:B:145:VAL:H    | 7        | 0.46          |
| (1,167)  | 1:A:81:VAL:H     | 1:A:141:GLY:HA2  | 6        | 0.46          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD11 | 5        | 0.46          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD12 | 5        | 0.46          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD13 | 5        | 0.46          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD21 | 5        | 0.46          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD22 | 5        | 0.46          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD23 | 5        | 0.46          |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB2  | 4        | 0.46          |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB3  | 4        | 0.46          |
| (1,158)  | 1:A:81:VAL:H     | 1:A:81:VAL:HB    | 2        | 0.46          |
| (1,158)  | 1:A:81:VAL:H     | 1:A:81:VAL:HB    | 6        | 0.46          |
| (1,158)  | 1:A:81:VAL:H     | 1:A:81:VAL:HB    | 9        | 0.46          |
| (1,1500) | 1:B:124:ILE:HA   | 1:B:124:ILE:H    | 3        | 0.46          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG12 | 4        | 0.46          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG13 | 4        | 0.46          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG12 | 4        | 0.46          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG13 | 4        | 0.46          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG12 | 4        | 0.46          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG13 | 4        | 0.46          |
| (1,1453) | 1:B:121:LYS:HA   | 1:B:122:TYR:H    | 6        | 0.46          |
| (1,1429) | 1:B:118:PHE:HA   | 1:B:118:PHE:H    | 7        | 0.46          |
| (1,1376) | 1:B:114:ILE:HG21 | 1:B:109:ASP:H    | 3        | 0.46          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1376) | 1:B:114:ILE:HG22 | 1:B:109:ASP:H   | 3        | 0.46          |
| (1,1376) | 1:B:114:ILE:HG23 | 1:B:109:ASP:H   | 3        | 0.46          |
| (1,1358) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3 | 5        | 0.46          |
| (1,1356) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3 | 5        | 0.46          |
| (1,1355) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB2 | 2        | 0.46          |
| (1,1355) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB2 | 5        | 0.46          |
| (1,1355) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB2 | 6        | 0.46          |
| (1,1297) | 1:B:107:ARG:H    | 1:B:108:GLN:H   | 9        | 0.46          |
| (1,1274) | 1:B:104:HIS:HA   | 1:B:105:GLU:H   | 1        | 0.46          |
| (1,1243) | 1:B:101:HIS:HB2  | 1:B:101:HIS:HD2 | 4        | 0.46          |
| (1,1232) | 1:B:100:VAL:HG11 | 1:B:102:GLY:H   | 9        | 0.46          |
| (1,1232) | 1:B:100:VAL:HG12 | 1:B:102:GLY:H   | 9        | 0.46          |
| (1,1232) | 1:B:100:VAL:HG13 | 1:B:102:GLY:H   | 9        | 0.46          |
| (1,1213) | 1:B:98:ILE:H     | 1:B:122:TYR:H   | 7        | 0.46          |
| (1,1212) | 1:B:98:ILE:H     | 1:B:122:TYR:H   | 7        | 0.46          |
| (1,1204) | 1:B:98:ILE:HD11  | 1:B:98:ILE:HB   | 8        | 0.46          |
| (1,1204) | 1:B:98:ILE:HD12  | 1:B:98:ILE:HB   | 8        | 0.46          |
| (1,1204) | 1:B:98:ILE:HD13  | 1:B:98:ILE:HB   | 8        | 0.46          |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD11 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD12 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD13 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD21 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD22 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD23 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD11 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD12 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD13 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD21 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD22 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE2   | 1:A:70:LEU:HD23 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD11 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD12 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD13 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD21 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD22 | 3        | 0.46          |
| (1,12)   | 1:A:68:MET:HE3   | 1:A:70:LEU:HD23 | 3        | 0.46          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB2  | 5        | 0.46          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB3  | 5        | 0.46          |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB2  | 6        | 0.46          |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB3  | 6        | 0.46          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD11 | 5        | 0.46          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD12 | 5        | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD13  | 5        | 0.46          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD21  | 5        | 0.46          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD22  | 5        | 0.46          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD23  | 5        | 0.46          |
| (1,1154) | 1:B:93:VAL:HA    | 1:B:98:ILE:HA    | 8        | 0.46          |
| (1,1154) | 1:B:93:VAL:HA    | 1:B:98:ILE:HA    | 9        | 0.46          |
| (1,1126) | 1:B:89:LEU:HD11  | 1:B:103:LYS:H    | 9        | 0.46          |
| (1,1126) | 1:B:89:LEU:HD12  | 1:B:103:LYS:H    | 9        | 0.46          |
| (1,1126) | 1:B:89:LEU:HD13  | 1:B:103:LYS:H    | 9        | 0.46          |
| (1,107)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:HG    | 7        | 0.46          |
| (1,107)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:HG    | 7        | 0.46          |
| (1,107)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:HG    | 7        | 0.46          |
| (1,1051) | 1:B:83:HIS:H     | 1:B:84:PHE:H     | 3        | 0.46          |
| (1,1050) | 1:B:83:HIS:H     | 1:B:84:PHE:H     | 3        | 0.46          |
| (1,1046) | 1:B:83:HIS:HA    | 1:B:83:HIS:H     | 2        | 0.46          |
| (1,1025) | 1:B:81:VAL:H     | 1:B:81:VAL:HB    | 2        | 0.46          |
| (1,1025) | 1:B:81:VAL:H     | 1:B:81:VAL:HB    | 6        | 0.46          |
| (1,1025) | 1:B:81:VAL:H     | 1:B:81:VAL:HB    | 9        | 0.46          |
| (1,986)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB3  | 8        | 0.45          |
| (1,979)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HD1  | 3        | 0.45          |
| (1,979)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HD2  | 3        | 0.45          |
| (1,979)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HD1  | 3        | 0.45          |
| (1,979)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HD2  | 3        | 0.45          |
| (1,979)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HD1  | 3        | 0.45          |
| (1,979)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HD2  | 3        | 0.45          |
| (1,929)  | 1:B:76:SER:HB3   | 1:B:76:SER:H     | 8        | 0.45          |
| (1,870)  | 1:B:66:SER:HB2   | 1:B:66:SER:H     | 3        | 0.45          |
| (1,819)  | 1:A:145:VAL:HG21 | 1:A:145:VAL:H    | 4        | 0.45          |
| (1,819)  | 1:A:145:VAL:HG22 | 1:A:145:VAL:H    | 4        | 0.45          |
| (1,819)  | 1:A:145:VAL:HG23 | 1:A:145:VAL:H    | 4        | 0.45          |
| (1,812)  | 1:A:145:VAL:HB   | 1:A:135:SER:HA   | 3        | 0.45          |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB2  | 2        | 0.45          |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB3  | 2        | 0.45          |
| (1,744)  | 1:A:135:SER:HB3  | 1:A:146:ASP:H    | 2        | 0.45          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG11 | 3        | 0.45          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG12 | 3        | 0.45          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG13 | 3        | 0.45          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG21 | 3        | 0.45          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG22 | 3        | 0.45          |
| (1,674)  | 1:A:127:ASP:H    | 1:A:128:VAL:HG23 | 3        | 0.45          |
| (1,673)  | 1:A:127:ASP:HB3  | 1:A:128:VAL:H    | 6        | 0.45          |
| (1,633)  | 1:A:124:ILE:HA   | 1:A:124:ILE:H    | 2        | 0.45          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,62)   | 1:A:76:SER:HB3  | 1:A:76:SER:H     | 8        | 0.45          |
| (1,590)  | 1:A:122:TYR:HA  | 1:A:98:ILE:H     | 3        | 0.45          |
| (1,590)  | 1:A:122:TYR:HA  | 1:A:98:ILE:H     | 7        | 0.45          |
| (1,586)  | 1:A:121:LYS:HA  | 1:A:122:TYR:H    | 8        | 0.45          |
| (1,566)  | 1:A:118:PHE:HA  | 1:A:119:HIS:H    | 3        | 0.45          |
| (1,562)  | 1:A:118:PHE:HA  | 1:A:118:PHE:H    | 4        | 0.45          |
| (1,562)  | 1:A:118:PHE:HA  | 1:A:118:PHE:H    | 6        | 0.45          |
| (1,539)  | 1:A:116:ARG:H   | 1:A:116:ARG:HG2  | 7        | 0.45          |
| (1,539)  | 1:A:116:ARG:H   | 1:A:116:ARG:HG3  | 7        | 0.45          |
| (1,524)  | 1:A:115:SER:HB2 | 1:A:106:GLU:H    | 5        | 0.45          |
| (1,498)  | 1:A:113:PHE:HB2 | 1:A:113:PHE:H    | 9        | 0.45          |
| (1,473)  | 1:A:111:HIS:HB3 | 1:A:114:ILE:HG21 | 6        | 0.45          |
| (1,473)  | 1:A:111:HIS:HB3 | 1:A:114:ILE:HG22 | 6        | 0.45          |
| (1,473)  | 1:A:111:HIS:HB3 | 1:A:114:ILE:HG23 | 6        | 0.45          |
| (1,447)  | 1:A:109:ASP:H   | 1:A:109:ASP:HB2  | 2        | 0.45          |
| (1,447)  | 1:A:109:ASP:H   | 1:A:109:ASP:HB3  | 2        | 0.45          |
| (1,407)  | 1:A:104:HIS:HA  | 1:A:105:GLU:H    | 6        | 0.45          |
| (1,383)  | 1:A:101:HIS:HA  | 1:A:119:HIS:HD2  | 1        | 0.45          |
| (1,376)  | 1:A:101:HIS:HB2 | 1:A:101:HIS:HD2  | 7        | 0.45          |
| (1,301)  | 1:A:95:GLY:H    | 1:A:94:LEU:HG    | 9        | 0.45          |
| (1,3)    | 1:A:66:SER:HB2  | 1:A:66:SER:H     | 3        | 0.45          |
| (1,252)  | 1:A:89:LEU:H    | 1:A:90:LYS:H     | 5        | 0.45          |
| (1,231)  | 1:A:87:GLU:HB2  | 1:A:89:LEU:H     | 4        | 0.45          |
| (1,231)  | 1:A:87:GLU:HB3  | 1:A:89:LEU:H     | 4        | 0.45          |
| (1,231)  | 1:A:87:GLU:HB2  | 1:A:89:LEU:H     | 7        | 0.45          |
| (1,231)  | 1:A:87:GLU:HB3  | 1:A:89:LEU:H     | 7        | 0.45          |
| (1,228)  | 1:A:87:GLU:H    | 1:A:88:GLU:H     | 5        | 0.45          |
| (1,225)  | 1:A:87:GLU:H    | 1:A:88:GLU:H     | 5        | 0.45          |
| (1,218)  | 1:A:86:PRO:HB2  | 1:A:85:SER:HA    | 3        | 0.45          |
| (1,218)  | 1:A:86:PRO:HB3  | 1:A:85:SER:HA    | 3        | 0.45          |
| (1,212)  | 1:A:85:SER:HB2  | 1:A:88:GLU:H     | 6        | 0.45          |
| (1,199)  | 1:A:84:PHE:HB2  | 1:A:85:SER:H     | 6        | 0.45          |
| (1,199)  | 1:A:84:PHE:HB3  | 1:A:85:SER:H     | 6        | 0.45          |
| (1,163)  | 1:A:81:VAL:HG21 | 1:A:83:HIS:H     | 1        | 0.45          |
| (1,163)  | 1:A:81:VAL:HG22 | 1:A:83:HIS:H     | 1        | 0.45          |
| (1,163)  | 1:A:81:VAL:HG23 | 1:A:83:HIS:H     | 1        | 0.45          |
| (1,1619) | 1:B:137:LEU:H   | 1:B:137:LEU:HB2  | 2        | 0.45          |
| (1,1619) | 1:B:137:LEU:H   | 1:B:137:LEU:HB3  | 2        | 0.45          |
| (1,1619) | 1:B:137:LEU:H   | 1:B:137:LEU:HB2  | 8        | 0.45          |
| (1,1619) | 1:B:137:LEU:H   | 1:B:137:LEU:HB3  | 8        | 0.45          |
| (1,1611) | 1:B:135:SER:HB3 | 1:B:146:ASP:H    | 2        | 0.45          |
| (1,1541) | 1:B:127:ASP:H   | 1:B:128:VAL:HG11 | 3        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG12 | 3        | 0.45          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG13 | 3        | 0.45          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG21 | 3        | 0.45          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG22 | 3        | 0.45          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG23 | 3        | 0.45          |
| (1,1540) | 1:B:127:ASP:HB3  | 1:B:128:VAL:H    | 6        | 0.45          |
| (1,1500) | 1:B:124:ILE:HA   | 1:B:124:ILE:H    | 2        | 0.45          |
| (1,1488) | 1:B:124:ILE:HD11 | 1:B:123:ARG:HA   | 2        | 0.45          |
| (1,1488) | 1:B:124:ILE:HD12 | 1:B:123:ARG:HA   | 2        | 0.45          |
| (1,1488) | 1:B:124:ILE:HD13 | 1:B:123:ARG:HA   | 2        | 0.45          |
| (1,1457) | 1:B:122:TYR:HA   | 1:B:98:ILE:H     | 3        | 0.45          |
| (1,1457) | 1:B:122:TYR:HA   | 1:B:98:ILE:H     | 7        | 0.45          |
| (1,1453) | 1:B:121:LYS:HA   | 1:B:122:TYR:H    | 8        | 0.45          |
| (1,1441) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HD2  | 9        | 0.45          |
| (1,1438) | 1:B:119:HIS:HA   | 1:B:101:HIS:HD2  | 3        | 0.45          |
| (1,1433) | 1:B:118:PHE:HA   | 1:B:119:HIS:H    | 3        | 0.45          |
| (1,1429) | 1:B:118:PHE:HA   | 1:B:118:PHE:H    | 4        | 0.45          |
| (1,1429) | 1:B:118:PHE:HA   | 1:B:118:PHE:H    | 6        | 0.45          |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG2  | 7        | 0.45          |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG3  | 7        | 0.45          |
| (1,1391) | 1:B:115:SER:HB2  | 1:B:106:GLU:H    | 5        | 0.45          |
| (1,1365) | 1:B:113:PHE:HB2  | 1:B:113:PHE:H    | 9        | 0.45          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG21 | 6        | 0.45          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG22 | 6        | 0.45          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG23 | 6        | 0.45          |
| (1,1274) | 1:B:104:HIS:HA   | 1:B:105:GLU:H    | 6        | 0.45          |
| (1,119)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB3  | 8        | 0.45          |
| (1,1168) | 1:B:95:GLY:H     | 1:B:94:LEU:HG    | 9        | 0.45          |
| (1,1152) | 1:B:93:VAL:HG11  | 1:B:93:VAL:H     | 5        | 0.45          |
| (1,1152) | 1:B:93:VAL:HG12  | 1:B:93:VAL:H     | 5        | 0.45          |
| (1,1152) | 1:B:93:VAL:HG13  | 1:B:93:VAL:H     | 5        | 0.45          |
| (1,1152) | 1:B:93:VAL:HG21  | 1:B:93:VAL:H     | 5        | 0.45          |
| (1,1152) | 1:B:93:VAL:HG22  | 1:B:93:VAL:H     | 5        | 0.45          |
| (1,1152) | 1:B:93:VAL:HG23  | 1:B:93:VAL:H     | 5        | 0.45          |
| (1,112)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HD1  | 3        | 0.45          |
| (1,112)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HD2  | 3        | 0.45          |
| (1,112)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HD1  | 3        | 0.45          |
| (1,112)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HD2  | 3        | 0.45          |
| (1,112)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HD1  | 3        | 0.45          |
| (1,112)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HD2  | 3        | 0.45          |
| (1,1119) | 1:B:89:LEU:H     | 1:B:90:LYS:H     | 5        | 0.45          |
| (1,1098) | 1:B:87:GLU:HB2   | 1:B:89:LEU:H     | 4        | 0.45          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1098) | 1:B:87:GLU:HB3  | 1:B:89:LEU:H     | 4        | 0.45          |
| (1,1095) | 1:B:87:GLU:H    | 1:B:88:GLU:H     | 5        | 0.45          |
| (1,1092) | 1:B:87:GLU:H    | 1:B:88:GLU:H     | 5        | 0.45          |
| (1,1079) | 1:B:85:SER:HB2  | 1:B:88:GLU:H     | 6        | 0.45          |
| (1,1066) | 1:B:84:PHE:HB2  | 1:B:85:SER:H     | 6        | 0.45          |
| (1,1066) | 1:B:84:PHE:HB3  | 1:B:85:SER:H     | 6        | 0.45          |
| (1,1034) | 1:B:81:VAL:H    | 1:B:141:GLY:HA2  | 6        | 0.45          |
| (1,1030) | 1:B:81:VAL:HG21 | 1:B:83:HIS:H     | 1        | 0.45          |
| (1,1030) | 1:B:81:VAL:HG22 | 1:B:83:HIS:H     | 1        | 0.45          |
| (1,1030) | 1:B:81:VAL:HG23 | 1:B:83:HIS:H     | 1        | 0.45          |
| (1,979)  | 1:B:77:VAL:HG11 | 1:B:122:TYR:HD1  | 4        | 0.44          |
| (1,979)  | 1:B:77:VAL:HG11 | 1:B:122:TYR:HD2  | 4        | 0.44          |
| (1,979)  | 1:B:77:VAL:HG12 | 1:B:122:TYR:HD1  | 4        | 0.44          |
| (1,979)  | 1:B:77:VAL:HG12 | 1:B:122:TYR:HD2  | 4        | 0.44          |
| (1,979)  | 1:B:77:VAL:HG13 | 1:B:122:TYR:HD1  | 4        | 0.44          |
| (1,979)  | 1:B:77:VAL:HG13 | 1:B:122:TYR:HD2  | 4        | 0.44          |
| (1,972)  | 1:B:77:VAL:HG21 | 1:B:79:LEU:HG    | 1        | 0.44          |
| (1,972)  | 1:B:77:VAL:HG22 | 1:B:79:LEU:HG    | 1        | 0.44          |
| (1,972)  | 1:B:77:VAL:HG23 | 1:B:79:LEU:HG    | 1        | 0.44          |
| (1,955)  | 1:B:77:VAL:HG11 | 1:B:76:SER:HA    | 5        | 0.44          |
| (1,955)  | 1:B:77:VAL:HG12 | 1:B:76:SER:HA    | 5        | 0.44          |
| (1,955)  | 1:B:77:VAL:HG13 | 1:B:76:SER:HA    | 5        | 0.44          |
| (1,955)  | 1:B:77:VAL:HG11 | 1:B:76:SER:HA    | 7        | 0.44          |
| (1,955)  | 1:B:77:VAL:HG12 | 1:B:76:SER:HA    | 7        | 0.44          |
| (1,955)  | 1:B:77:VAL:HG13 | 1:B:76:SER:HA    | 7        | 0.44          |
| (1,898)  | 1:B:73:ASP:H    | 1:B:72:LYS:HB2   | 2        | 0.44          |
| (1,898)  | 1:B:73:ASP:H    | 1:B:72:LYS:HB3   | 2        | 0.44          |
| (1,88)   | 1:A:77:VAL:HG11 | 1:A:76:SER:HA    | 7        | 0.44          |
| (1,88)   | 1:A:77:VAL:HG12 | 1:A:76:SER:HA    | 7        | 0.44          |
| (1,88)   | 1:A:77:VAL:HG13 | 1:A:76:SER:HA    | 7        | 0.44          |
| (1,843)  | 1:A:147:GLY:HA2 | 1:A:133:ILE:HB   | 8        | 0.44          |
| (1,798)  | 1:A:144:THR:H   | 1:A:143:LEU:HD11 | 6        | 0.44          |
| (1,798)  | 1:A:144:THR:H   | 1:A:143:LEU:HD12 | 6        | 0.44          |
| (1,798)  | 1:A:144:THR:H   | 1:A:143:LEU:HD13 | 6        | 0.44          |
| (1,798)  | 1:A:144:THR:H   | 1:A:143:LEU:HD21 | 6        | 0.44          |
| (1,798)  | 1:A:144:THR:H   | 1:A:143:LEU:HD22 | 6        | 0.44          |
| (1,798)  | 1:A:144:THR:H   | 1:A:143:LEU:HD23 | 6        | 0.44          |
| (1,791)  | 1:A:143:LEU:HA  | 1:A:144:THR:H    | 1        | 0.44          |
| (1,791)  | 1:A:143:LEU:HA  | 1:A:144:THR:H    | 2        | 0.44          |
| (1,791)  | 1:A:143:LEU:HA  | 1:A:144:THR:H    | 3        | 0.44          |
| (1,752)  | 1:A:137:LEU:H   | 1:A:137:LEU:HB2  | 1        | 0.44          |
| (1,752)  | 1:A:137:LEU:H   | 1:A:137:LEU:HB3  | 1        | 0.44          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,635) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 8        | 0.44          |
| (1,635) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 8        | 0.44          |
| (1,635) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 8        | 0.44          |
| (1,634) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 8        | 0.44          |
| (1,634) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 8        | 0.44          |
| (1,634) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 8        | 0.44          |
| (1,633) | 1:A:124:ILE:HA   | 1:A:124:ILE:H    | 1        | 0.44          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG12 | 3        | 0.44          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG13 | 3        | 0.44          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG12 | 3        | 0.44          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG13 | 3        | 0.44          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG12 | 3        | 0.44          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG13 | 3        | 0.44          |
| (1,621) | 1:A:124:ILE:HD11 | 1:A:123:ARG:HA   | 2        | 0.44          |
| (1,621) | 1:A:124:ILE:HD12 | 1:A:123:ARG:HA   | 2        | 0.44          |
| (1,621) | 1:A:124:ILE:HD13 | 1:A:123:ARG:HA   | 2        | 0.44          |
| (1,574) | 1:A:119:HIS:HB3  | 1:A:119:HIS:HD2  | 5        | 0.44          |
| (1,566) | 1:A:118:PHE:HA   | 1:A:119:HIS:H    | 9        | 0.44          |
| (1,562) | 1:A:118:PHE:HA   | 1:A:118:PHE:H    | 5        | 0.44          |
| (1,547) | 1:A:117:GLU:H    | 1:A:117:GLU:HG2  | 7        | 0.44          |
| (1,547) | 1:A:117:GLU:H    | 1:A:117:GLU:HG3  | 7        | 0.44          |
| (1,512) | 1:A:114:ILE:HD11 | 1:A:113:PHE:HA   | 3        | 0.44          |
| (1,512) | 1:A:114:ILE:HD12 | 1:A:113:PHE:HA   | 3        | 0.44          |
| (1,512) | 1:A:114:ILE:HD13 | 1:A:113:PHE:HA   | 3        | 0.44          |
| (1,491) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 4        | 0.44          |
| (1,489) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 4        | 0.44          |
| (1,465) | 1:A:111:HIS:HB2  | 1:A:111:HIS:H    | 4        | 0.44          |
| (1,445) | 1:A:108:GLN:HA   | 1:A:113:PHE:H    | 1        | 0.44          |
| (1,368) | 1:A:101:HIS:HB2  | 1:A:92:LYS:HB2   | 7        | 0.44          |
| (1,368) | 1:A:101:HIS:HB2  | 1:A:92:LYS:HB3   | 7        | 0.44          |
| (1,367) | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB2   | 7        | 0.44          |
| (1,367) | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB3   | 7        | 0.44          |
| (1,337) | 1:A:98:ILE:HD11  | 1:A:98:ILE:HB    | 7        | 0.44          |
| (1,337) | 1:A:98:ILE:HD12  | 1:A:98:ILE:HB    | 7        | 0.44          |
| (1,337) | 1:A:98:ILE:HD13  | 1:A:98:ILE:HB    | 7        | 0.44          |
| (1,323) | 1:A:97:VAL:HB    | 1:A:94:LEU:HB2   | 7        | 0.44          |
| (1,323) | 1:A:97:VAL:HB    | 1:A:94:LEU:HB3   | 7        | 0.44          |
| (1,297) | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD11  | 9        | 0.44          |
| (1,297) | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD12  | 9        | 0.44          |
| (1,297) | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD13  | 9        | 0.44          |
| (1,297) | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD21  | 9        | 0.44          |
| (1,297) | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD22  | 9        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD23  | 9        | 0.44          |
| (1,252)  | 1:A:89:LEU:H     | 1:A:90:LYS:H     | 7        | 0.44          |
| (1,239)  | 1:A:89:LEU:H     | 1:A:87:GLU:HA    | 4        | 0.44          |
| (1,231)  | 1:A:87:GLU:HB2   | 1:A:89:LEU:H     | 8        | 0.44          |
| (1,231)  | 1:A:87:GLU:HB3   | 1:A:89:LEU:H     | 8        | 0.44          |
| (1,1710) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HB   | 8        | 0.44          |
| (1,1686) | 1:B:145:VAL:HG21 | 1:B:145:VAL:H    | 4        | 0.44          |
| (1,1686) | 1:B:145:VAL:HG22 | 1:B:145:VAL:H    | 4        | 0.44          |
| (1,1686) | 1:B:145:VAL:HG23 | 1:B:145:VAL:H    | 4        | 0.44          |
| (1,1679) | 1:B:145:VAL:HB   | 1:B:135:SER:HA   | 3        | 0.44          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD11 | 6        | 0.44          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD12 | 6        | 0.44          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD13 | 6        | 0.44          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD21 | 6        | 0.44          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD22 | 6        | 0.44          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD23 | 6        | 0.44          |
| (1,1658) | 1:B:143:LEU:HA   | 1:B:144:THR:H    | 1        | 0.44          |
| (1,1658) | 1:B:143:LEU:HA   | 1:B:144:THR:H    | 3        | 0.44          |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB2  | 1        | 0.44          |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB3  | 1        | 0.44          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG21 | 6        | 0.44          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG22 | 6        | 0.44          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG23 | 6        | 0.44          |
| (1,1500) | 1:B:124:ILE:HA   | 1:B:124:ILE:H    | 1        | 0.44          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG12 | 3        | 0.44          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG13 | 3        | 0.44          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG12 | 3        | 0.44          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG13 | 3        | 0.44          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG12 | 3        | 0.44          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG13 | 3        | 0.44          |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD11  | 4        | 0.44          |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD12  | 4        | 0.44          |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD13  | 4        | 0.44          |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD11  | 4        | 0.44          |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD12  | 4        | 0.44          |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD13  | 4        | 0.44          |
| (1,1433) | 1:B:118:PHE:HA   | 1:B:119:HIS:H    | 9        | 0.44          |
| (1,1429) | 1:B:118:PHE:HA   | 1:B:118:PHE:H    | 5        | 0.44          |
| (1,1414) | 1:B:117:GLU:H    | 1:B:117:GLU:HG2  | 7        | 0.44          |
| (1,1414) | 1:B:117:GLU:H    | 1:B:117:GLU:HG3  | 7        | 0.44          |
| (1,1379) | 1:B:114:ILE:HD11 | 1:B:113:PHE:HA   | 3        | 0.44          |
| (1,1379) | 1:B:114:ILE:HD12 | 1:B:113:PHE:HA   | 3        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1379) | 1:B:114:ILE:HD13 | 1:B:113:PHE:HA   | 3        | 0.44          |
| (1,1332) | 1:B:111:HIS:HB2  | 1:B:111:HIS:H    | 4        | 0.44          |
| (1,1314) | 1:B:109:ASP:H    | 1:B:109:ASP:HB2  | 2        | 0.44          |
| (1,1314) | 1:B:109:ASP:H    | 1:B:109:ASP:HB3  | 2        | 0.44          |
| (1,1312) | 1:B:108:GLN:HA   | 1:B:113:PHE:H    | 1        | 0.44          |
| (1,1235) | 1:B:101:HIS:HB2  | 1:B:92:LYS:HB2   | 7        | 0.44          |
| (1,1235) | 1:B:101:HIS:HB2  | 1:B:92:LYS:HB3   | 7        | 0.44          |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB2   | 7        | 0.44          |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB3   | 7        | 0.44          |
| (1,1204) | 1:B:98:ILE:HD11  | 1:B:98:ILE:HB    | 7        | 0.44          |
| (1,1204) | 1:B:98:ILE:HD12  | 1:B:98:ILE:HB    | 7        | 0.44          |
| (1,1204) | 1:B:98:ILE:HD13  | 1:B:98:ILE:HB    | 7        | 0.44          |
| (1,1199) | 1:B:97:VAL:HA    | 1:B:124:ILE:HG12 | 8        | 0.44          |
| (1,1199) | 1:B:97:VAL:HA    | 1:B:124:ILE:HG13 | 8        | 0.44          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB2   | 7        | 0.44          |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB3   | 7        | 0.44          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD11  | 9        | 0.44          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD12  | 9        | 0.44          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD13  | 9        | 0.44          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD21  | 9        | 0.44          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD22  | 9        | 0.44          |
| (1,1164) | 1:B:95:GLY:HA2   | 1:B:94:LEU:HD23  | 9        | 0.44          |
| (1,112)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HD1  | 4        | 0.44          |
| (1,112)  | 1:A:77:VAL:HG11  | 1:A:122:TYR:HD2  | 4        | 0.44          |
| (1,112)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HD1  | 4        | 0.44          |
| (1,112)  | 1:A:77:VAL:HG12  | 1:A:122:TYR:HD2  | 4        | 0.44          |
| (1,112)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HD1  | 4        | 0.44          |
| (1,112)  | 1:A:77:VAL:HG13  | 1:A:122:TYR:HD2  | 4        | 0.44          |
| (1,1119) | 1:B:89:LEU:H     | 1:B:90:LYS:H     | 7        | 0.44          |
| (1,1106) | 1:B:89:LEU:H     | 1:B:87:GLU:HA    | 4        | 0.44          |
| (1,1098) | 1:B:87:GLU:HB2   | 1:B:89:LEU:H     | 7        | 0.44          |
| (1,1098) | 1:B:87:GLU:HB3   | 1:B:89:LEU:H     | 7        | 0.44          |
| (1,1098) | 1:B:87:GLU:HB2   | 1:B:89:LEU:H     | 8        | 0.44          |
| (1,1098) | 1:B:87:GLU:HB3   | 1:B:89:LEU:H     | 8        | 0.44          |
| (1,1085) | 1:B:86:PRO:HB2   | 1:B:85:SER:HA    | 3        | 0.44          |
| (1,1085) | 1:B:86:PRO:HB3   | 1:B:85:SER:HA    | 3        | 0.44          |
| (1,105)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HG    | 1        | 0.44          |
| (1,105)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HG    | 1        | 0.44          |
| (1,105)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HG    | 1        | 0.44          |
| (1,923)  | 1:B:75:PHE:HD1   | 1:B:148:PRO:HA   | 6        | 0.43          |
| (1,923)  | 1:B:75:PHE:HD2   | 1:B:148:PRO:HA   | 6        | 0.43          |
| (1,913)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HB2   | 6        | 0.43          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,913) | 1:B:75:PHE:HA    | 1:B:75:PHE:HB2   | 8        | 0.43          |
| (1,893) | 1:B:71:GLU:H     | 1:B:76:SER:H     | 2        | 0.43          |
| (1,891) | 1:B:71:GLU:H     | 1:B:69:ARG:HG2   | 5        | 0.43          |
| (1,891) | 1:B:71:GLU:H     | 1:B:69:ARG:HG3   | 5        | 0.43          |
| (1,880) | 1:B:68:MET:HE1   | 1:B:122:TYR:HE1  | 7        | 0.43          |
| (1,880) | 1:B:68:MET:HE1   | 1:B:122:TYR:HE2  | 7        | 0.43          |
| (1,880) | 1:B:68:MET:HE2   | 1:B:122:TYR:HE1  | 7        | 0.43          |
| (1,880) | 1:B:68:MET:HE2   | 1:B:122:TYR:HE2  | 7        | 0.43          |
| (1,880) | 1:B:68:MET:HE3   | 1:B:122:TYR:HE1  | 7        | 0.43          |
| (1,880) | 1:B:68:MET:HE3   | 1:B:122:TYR:HE2  | 7        | 0.43          |
| (1,88)  | 1:A:77:VAL:HG11  | 1:A:76:SER:HA    | 5        | 0.43          |
| (1,88)  | 1:A:77:VAL:HG12  | 1:A:76:SER:HA    | 5        | 0.43          |
| (1,88)  | 1:A:77:VAL:HG13  | 1:A:76:SER:HA    | 5        | 0.43          |
| (1,854) | 1:A:148:PRO:HB2  | 1:A:149:ARG:H    | 1        | 0.43          |
| (1,854) | 1:A:148:PRO:HB3  | 1:A:149:ARG:H    | 1        | 0.43          |
| (1,848) | 1:A:147:GLY:HA3  | 1:A:147:GLY:H    | 3        | 0.43          |
| (1,843) | 1:A:147:GLY:HA2  | 1:A:133:ILE:HB   | 7        | 0.43          |
| (1,791) | 1:A:143:LEU:HA   | 1:A:144:THR:H    | 4        | 0.43          |
| (1,791) | 1:A:143:LEU:HA   | 1:A:144:THR:H    | 6        | 0.43          |
| (1,791) | 1:A:143:LEU:HA   | 1:A:144:THR:H    | 7        | 0.43          |
| (1,791) | 1:A:143:LEU:HA   | 1:A:144:THR:H    | 8        | 0.43          |
| (1,791) | 1:A:143:LEU:HA   | 1:A:144:THR:H    | 9        | 0.43          |
| (1,783) | 1:A:142:VAL:HG11 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,783) | 1:A:142:VAL:HG12 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,783) | 1:A:142:VAL:HG13 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,783) | 1:A:142:VAL:HG21 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,783) | 1:A:142:VAL:HG22 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,783) | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,782) | 1:A:142:VAL:HG11 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,782) | 1:A:142:VAL:HG12 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,782) | 1:A:142:VAL:HG13 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,782) | 1:A:142:VAL:HG21 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,782) | 1:A:142:VAL:HG22 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,782) | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 9        | 0.43          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG21 | 6        | 0.43          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG22 | 6        | 0.43          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG23 | 6        | 0.43          |
| (1,700) | 1:A:132:THR:HG21 | 1:A:132:THR:H    | 7        | 0.43          |
| (1,700) | 1:A:132:THR:HG22 | 1:A:132:THR:H    | 7        | 0.43          |
| (1,700) | 1:A:132:THR:HG23 | 1:A:132:THR:H    | 7        | 0.43          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG12 | 6        | 0.43          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG13 | 6        | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,629)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG12 | 6        | 0.43          |
| (1,629)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG13 | 6        | 0.43          |
| (1,629)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG12 | 6        | 0.43          |
| (1,629)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG13 | 6        | 0.43          |
| (1,584)  | 1:A:121:LYS:HA   | 1:A:120:ARG:HB2  | 8        | 0.43          |
| (1,584)  | 1:A:121:LYS:HA   | 1:A:120:ARG:HB3  | 8        | 0.43          |
| (1,583)  | 1:A:121:LYS:HA   | 1:A:99:GLU:HA    | 2        | 0.43          |
| (1,579)  | 1:A:119:HIS:H    | 1:A:120:ARG:H    | 6        | 0.43          |
| (1,574)  | 1:A:119:HIS:HB3  | 1:A:119:HIS:HD2  | 9        | 0.43          |
| (1,562)  | 1:A:118:PHE:HA   | 1:A:118:PHE:H    | 3        | 0.43          |
| (1,56)   | 1:A:75:PHE:HD1   | 1:A:148:PRO:HA   | 6        | 0.43          |
| (1,56)   | 1:A:75:PHE:HD2   | 1:A:148:PRO:HA   | 6        | 0.43          |
| (1,46)   | 1:A:75:PHE:HA    | 1:A:75:PHE:HB2   | 8        | 0.43          |
| (1,407)  | 1:A:104:HIS:HA   | 1:A:105:GLU:H    | 8        | 0.43          |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG2   | 4        | 0.43          |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG3   | 4        | 0.43          |
| (1,358)  | 1:A:100:VAL:HG11 | 1:A:92:LYS:H     | 7        | 0.43          |
| (1,358)  | 1:A:100:VAL:HG12 | 1:A:92:LYS:H     | 7        | 0.43          |
| (1,358)  | 1:A:100:VAL:HG13 | 1:A:92:LYS:H     | 7        | 0.43          |
| (1,332)  | 1:A:97:VAL:HA    | 1:A:124:ILE:HG12 | 8        | 0.43          |
| (1,332)  | 1:A:97:VAL:HA    | 1:A:124:ILE:HG13 | 8        | 0.43          |
| (1,31)   | 1:A:73:ASP:H     | 1:A:72:LYS:HB2   | 2        | 0.43          |
| (1,31)   | 1:A:73:ASP:H     | 1:A:72:LYS:HB3   | 2        | 0.43          |
| (1,301)  | 1:A:95:GLY:H     | 1:A:94:LEU:HG    | 4        | 0.43          |
| (1,26)   | 1:A:71:GLU:H     | 1:A:76:SER:H     | 2        | 0.43          |
| (1,252)  | 1:A:89:LEU:H     | 1:A:90:LYS:H     | 4        | 0.43          |
| (1,251)  | 1:A:89:LEU:HG    | 1:A:90:LYS:H     | 3        | 0.43          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG2   | 5        | 0.43          |
| (1,24)   | 1:A:71:GLU:H     | 1:A:69:ARG:HG3   | 5        | 0.43          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB2   | 5        | 0.43          |
| (1,223)  | 1:A:87:GLU:H     | 1:A:88:GLU:HB3   | 5        | 0.43          |
| (1,193)  | 1:A:84:PHE:HD1   | 1:A:83:HIS:HA    | 7        | 0.43          |
| (1,193)  | 1:A:84:PHE:HD2   | 1:A:83:HIS:HA    | 7        | 0.43          |
| (1,185)  | 1:A:83:HIS:HB3   | 1:A:104:HIS:HB2  | 6        | 0.43          |
| (1,176)  | 1:A:83:HIS:HB3   | 1:A:83:HIS:HD2   | 3        | 0.43          |
| (1,1721) | 1:B:148:PRO:HB2  | 1:B:149:ARG:H    | 1        | 0.43          |
| (1,1721) | 1:B:148:PRO:HB3  | 1:B:149:ARG:H    | 1        | 0.43          |
| (1,1715) | 1:B:147:GLY:HA3  | 1:B:147:GLY:H    | 3        | 0.43          |
| (1,1710) | 1:B:147:GLY:HA2  | 1:B:133:ILE:HB   | 7        | 0.43          |
| (1,1658) | 1:B:143:LEU:HA   | 1:B:144:THR:H    | 2        | 0.43          |
| (1,1658) | 1:B:143:LEU:HA   | 1:B:144:THR:H    | 4        | 0.43          |
| (1,1658) | 1:B:143:LEU:HA   | 1:B:144:THR:H    | 6        | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1658) | 1:B:143:LEU:HA   | 1:B:144:THR:H    | 7        | 0.43          |
| (1,1658) | 1:B:143:LEU:HA   | 1:B:144:THR:H    | 8        | 0.43          |
| (1,1658) | 1:B:143:LEU:HA   | 1:B:144:THR:H    | 9        | 0.43          |
| (1,1567) | 1:B:132:THR:HG21 | 1:B:132:THR:H    | 7        | 0.43          |
| (1,1567) | 1:B:132:THR:HG22 | 1:B:132:THR:H    | 7        | 0.43          |
| (1,1567) | 1:B:132:THR:HG23 | 1:B:132:THR:H    | 7        | 0.43          |
| (1,155)  | 1:A:81:VAL:HG11  | 1:A:81:VAL:HA    | 4        | 0.43          |
| (1,155)  | 1:A:81:VAL:HG12  | 1:A:81:VAL:HA    | 4        | 0.43          |
| (1,155)  | 1:A:81:VAL:HG13  | 1:A:81:VAL:HA    | 4        | 0.43          |
| (1,1502) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 8        | 0.43          |
| (1,1502) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 8        | 0.43          |
| (1,1502) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H    | 8        | 0.43          |
| (1,1501) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 8        | 0.43          |
| (1,1501) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 8        | 0.43          |
| (1,1501) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H    | 8        | 0.43          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG12 | 6        | 0.43          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG13 | 6        | 0.43          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG12 | 6        | 0.43          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG13 | 6        | 0.43          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG12 | 6        | 0.43          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG13 | 6        | 0.43          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB2  | 8        | 0.43          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB3  | 8        | 0.43          |
| (1,1446) | 1:B:119:HIS:H    | 1:B:120:ARG:H    | 6        | 0.43          |
| (1,1429) | 1:B:118:PHE:HA   | 1:B:118:PHE:H    | 3        | 0.43          |
| (1,1358) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3  | 4        | 0.43          |
| (1,1356) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3  | 4        | 0.43          |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE1  | 7        | 0.43          |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE2  | 7        | 0.43          |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE1  | 7        | 0.43          |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE2  | 7        | 0.43          |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE1  | 7        | 0.43          |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE2  | 7        | 0.43          |
| (1,1274) | 1:B:104:HIS:HA   | 1:B:105:GLU:H    | 8        | 0.43          |
| (1,1260) | 1:B:103:LYS:H    | 1:B:88:GLU:HG2   | 4        | 0.43          |
| (1,1260) | 1:B:103:LYS:H    | 1:B:88:GLU:HG3   | 4        | 0.43          |
| (1,1225) | 1:B:100:VAL:HG11 | 1:B:92:LYS:H     | 7        | 0.43          |
| (1,1225) | 1:B:100:VAL:HG12 | 1:B:92:LYS:H     | 7        | 0.43          |
| (1,1225) | 1:B:100:VAL:HG13 | 1:B:92:LYS:H     | 7        | 0.43          |
| (1,1119) | 1:B:89:LEU:H     | 1:B:90:LYS:H     | 4        | 0.43          |
| (1,1118) | 1:B:89:LEU:HG    | 1:B:90:LYS:H     | 3        | 0.43          |
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB2   | 5        | 0.43          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1090) | 1:B:87:GLU:H     | 1:B:88:GLU:HB3  | 5        | 0.43          |
| (1,1060) | 1:B:84:PHE:HD1   | 1:B:83:HIS:HA   | 7        | 0.43          |
| (1,1060) | 1:B:84:PHE:HD2   | 1:B:83:HIS:HA   | 7        | 0.43          |
| (1,1052) | 1:B:83:HIS:HB3   | 1:B:104:HIS:HB2 | 6        | 0.43          |
| (1,1022) | 1:B:81:VAL:HG11  | 1:B:81:VAL:HA   | 4        | 0.43          |
| (1,1022) | 1:B:81:VAL:HG12  | 1:B:81:VAL:HA   | 4        | 0.43          |
| (1,1022) | 1:B:81:VAL:HG13  | 1:B:81:VAL:HA   | 4        | 0.43          |
| (1,982)  | 1:B:77:VAL:HG11  | 1:B:145:VAL:H   | 5        | 0.42          |
| (1,982)  | 1:B:77:VAL:HG12  | 1:B:145:VAL:H   | 5        | 0.42          |
| (1,982)  | 1:B:77:VAL:HG13  | 1:B:145:VAL:H   | 5        | 0.42          |
| (1,974)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HG   | 5        | 0.42          |
| (1,974)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HG   | 5        | 0.42          |
| (1,974)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HG   | 5        | 0.42          |
| (1,924)  | 1:B:75:PHE:H     | 1:B:149:ARG:H   | 8        | 0.42          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD11 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD12 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD13 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD21 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD22 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD23 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD11 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD12 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD13 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD21 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD22 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE2   | 1:B:70:LEU:HD23 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD11 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD12 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD13 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD21 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD22 | 9        | 0.42          |
| (1,879)  | 1:B:68:MET:HE3   | 1:B:70:LEU:HD23 | 9        | 0.42          |
| (1,857)  | 1:A:150:LYS:H    | 1:A:150:LYS:HD2 | 1        | 0.42          |
| (1,857)  | 1:A:150:LYS:H    | 1:A:150:LYS:HD3 | 1        | 0.42          |
| (1,839)  | 1:A:146:ASP:HB2  | 1:A:147:GLY:H   | 4        | 0.42          |
| (1,791)  | 1:A:143:LEU:HA   | 1:A:144:THR:H   | 5        | 0.42          |
| (1,714)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HA  | 3        | 0.42          |
| (1,714)  | 1:A:133:ILE:HD12 | 1:A:130:PRO:HA  | 3        | 0.42          |
| (1,714)  | 1:A:133:ILE:HD13 | 1:A:130:PRO:HA  | 3        | 0.42          |
| (1,635)  | 1:A:124:ILE:HD11 | 1:A:124:ILE:H   | 1        | 0.42          |
| (1,635)  | 1:A:124:ILE:HD12 | 1:A:124:ILE:H   | 1        | 0.42          |
| (1,635)  | 1:A:124:ILE:HD13 | 1:A:124:ILE:H   | 1        | 0.42          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,634) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 1        | 0.42          |
| (1,634) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 1        | 0.42          |
| (1,634) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 1        | 0.42          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG12 | 1        | 0.42          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG13 | 1        | 0.42          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG12 | 1        | 0.42          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG13 | 1        | 0.42          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG12 | 1        | 0.42          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG13 | 1        | 0.42          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG12 | 7        | 0.42          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG13 | 7        | 0.42          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG12 | 7        | 0.42          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG13 | 7        | 0.42          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG12 | 7        | 0.42          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG13 | 7        | 0.42          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG12 | 8        | 0.42          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG13 | 8        | 0.42          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG12 | 8        | 0.42          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG13 | 8        | 0.42          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG12 | 8        | 0.42          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG13 | 8        | 0.42          |
| (1,618) | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD1  | 1        | 0.42          |
| (1,618) | 1:A:124:ILE:HG21 | 1:A:122:TYR:HD2  | 1        | 0.42          |
| (1,618) | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD1  | 1        | 0.42          |
| (1,618) | 1:A:124:ILE:HG22 | 1:A:122:TYR:HD2  | 1        | 0.42          |
| (1,618) | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD1  | 1        | 0.42          |
| (1,618) | 1:A:124:ILE:HG23 | 1:A:122:TYR:HD2  | 1        | 0.42          |
| (1,585) | 1:A:121:LYS:HG2  | 1:A:121:LYS:HA   | 6        | 0.42          |
| (1,585) | 1:A:121:LYS:HG3  | 1:A:121:LYS:HA   | 6        | 0.42          |
| (1,585) | 1:A:121:LYS:HG2  | 1:A:121:LYS:HA   | 9        | 0.42          |
| (1,585) | 1:A:121:LYS:HG3  | 1:A:121:LYS:HA   | 9        | 0.42          |
| (1,573) | 1:A:119:HIS:HA   | 1:A:119:HIS:HD2  | 4        | 0.42          |
| (1,57)  | 1:A:75:PHE:H     | 1:A:149:ARG:H    | 8        | 0.42          |
| (1,544) | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 9        | 0.42          |
| (1,543) | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 9        | 0.42          |
| (1,488) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB2  | 8        | 0.42          |
| (1,470) | 1:A:111:HIS:HA   | 1:A:112:GLY:H    | 2        | 0.42          |
| (1,46)  | 1:A:75:PHE:HA    | 1:A:75:PHE:HB2   | 6        | 0.42          |
| (1,407) | 1:A:104:HIS:HA   | 1:A:105:GLU:H    | 5        | 0.42          |
| (1,407) | 1:A:104:HIS:HA   | 1:A:105:GLU:H    | 9        | 0.42          |
| (1,405) | 1:A:104:HIS:HB3  | 1:A:104:HIS:HA   | 7        | 0.42          |
| (1,404) | 1:A:104:HIS:HB3  | 1:A:104:HIS:HA   | 7        | 0.42          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG11 | 1        | 0.42          |
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG12 | 1        | 0.42          |
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG13 | 1        | 0.42          |
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG21 | 1        | 0.42          |
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG22 | 1        | 0.42          |
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG23 | 1        | 0.42          |
| (1,321)  | 1:A:97:VAL:H     | 1:A:93:VAL:HB   | 3        | 0.42          |
| (1,301)  | 1:A:95:GLY:H     | 1:A:94:LEU:HG   | 2        | 0.42          |
| (1,300)  | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB2  | 4        | 0.42          |
| (1,300)  | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB3  | 4        | 0.42          |
| (1,239)  | 1:A:89:LEU:H     | 1:A:87:GLU:HA   | 8        | 0.42          |
| (1,231)  | 1:A:87:GLU:HB2   | 1:A:89:LEU:H    | 6        | 0.42          |
| (1,231)  | 1:A:87:GLU:HB3   | 1:A:89:LEU:H    | 6        | 0.42          |
| (1,22)   | 1:A:70:LEU:HB3   | 1:A:74:ARG:H    | 8        | 0.42          |
| (1,189)  | 1:A:84:PHE:H     | 1:A:81:VAL:HB   | 1        | 0.42          |
| (1,1767) | 1:A:122:TYR:HB2  | 1:B:112:GLY:HA3 | 6        | 0.42          |
| (1,1767) | 1:A:122:TYR:HB3  | 1:B:112:GLY:HA3 | 6        | 0.42          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD2 | 1        | 0.42          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD3 | 1        | 0.42          |
| (1,1706) | 1:B:146:ASP:HB2  | 1:B:147:GLY:H   | 4        | 0.42          |
| (1,1658) | 1:B:143:LEU:HA   | 1:B:144:THR:H   | 5        | 0.42          |
| (1,1650) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1650) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1650) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1650) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1650) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1650) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1649) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1649) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1649) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1649) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1649) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1649) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H   | 9        | 0.42          |
| (1,1581) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HA  | 3        | 0.42          |
| (1,1581) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HA  | 3        | 0.42          |
| (1,1581) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HA  | 3        | 0.42          |
| (1,1502) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H   | 1        | 0.42          |
| (1,1502) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H   | 1        | 0.42          |
| (1,1502) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H   | 1        | 0.42          |
| (1,1501) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H   | 1        | 0.42          |
| (1,1501) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H   | 1        | 0.42          |
| (1,1501) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H   | 1        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG12 | 1        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG13 | 1        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG12 | 1        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG13 | 1        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG12 | 1        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG13 | 1        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG12 | 7        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG13 | 7        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG12 | 7        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG13 | 7        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG12 | 7        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG13 | 7        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG12 | 8        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG13 | 8        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG12 | 8        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG13 | 8        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG12 | 8        | 0.42          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG13 | 8        | 0.42          |
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD1  | 1        | 0.42          |
| (1,1485) | 1:B:124:ILE:HG21 | 1:B:122:TYR:HD2  | 1        | 0.42          |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD1  | 1        | 0.42          |
| (1,1485) | 1:B:124:ILE:HG22 | 1:B:122:TYR:HD2  | 1        | 0.42          |
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD1  | 1        | 0.42          |
| (1,1485) | 1:B:124:ILE:HG23 | 1:B:122:TYR:HD2  | 1        | 0.42          |
| (1,1452) | 1:B:121:LYS:HG2  | 1:B:121:LYS:HA   | 6        | 0.42          |
| (1,1452) | 1:B:121:LYS:HG3  | 1:B:121:LYS:HA   | 6        | 0.42          |
| (1,1452) | 1:B:121:LYS:HG2  | 1:B:121:LYS:HA   | 9        | 0.42          |
| (1,1452) | 1:B:121:LYS:HG3  | 1:B:121:LYS:HA   | 9        | 0.42          |
| (1,1450) | 1:B:121:LYS:HA   | 1:B:99:GLU:HA    | 2        | 0.42          |
| (1,1440) | 1:B:119:HIS:HA   | 1:B:119:HIS:HD2  | 4        | 0.42          |
| (1,1411) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA   | 9        | 0.42          |
| (1,1410) | 1:B:117:GLU:HA   | 1:B:103:LYS:HA   | 9        | 0.42          |
| (1,1355) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB2  | 8        | 0.42          |
| (1,1337) | 1:B:111:HIS:HA   | 1:B:112:GLY:H    | 2        | 0.42          |
| (1,1274) | 1:B:104:HIS:HA   | 1:B:105:GLU:H    | 5        | 0.42          |
| (1,1274) | 1:B:104:HIS:HA   | 1:B:105:GLU:H    | 9        | 0.42          |
| (1,1272) | 1:B:104:HIS:HB3  | 1:B:104:HIS:HA   | 7        | 0.42          |
| (1,1271) | 1:B:104:HIS:HB3  | 1:B:104:HIS:HA   | 7        | 0.42          |
| (1,1204) | 1:B:98:ILE:HD11  | 1:B:98:ILE:HB    | 4        | 0.42          |
| (1,1204) | 1:B:98:ILE:HD12  | 1:B:98:ILE:HB    | 4        | 0.42          |
| (1,1204) | 1:B:98:ILE:HD13  | 1:B:98:ILE:HB    | 4        | 0.42          |
| (1,12)   | 1:A:68:MET:HE1   | 1:A:70:LEU:HD11  | 9        | 0.42          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD12 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD13 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD21 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD22 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD23 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD11 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD12 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD13 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD21 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD22 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD23 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD11 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD12 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD13 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD21 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD22 | 9        | 0.42          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD23 | 9        | 0.42          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG11 | 1        | 0.42          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG12 | 1        | 0.42          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG13 | 1        | 0.42          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG21 | 1        | 0.42          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG22 | 1        | 0.42          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG23 | 1        | 0.42          |
| (1,1188) | 1:B:97:VAL:H    | 1:B:93:VAL:HB   | 3        | 0.42          |
| (1,1168) | 1:B:95:GLY:H    | 1:B:94:LEU:HG   | 2        | 0.42          |
| (1,1168) | 1:B:95:GLY:H    | 1:B:94:LEU:HG   | 4        | 0.42          |
| (1,1168) | 1:B:95:GLY:H    | 1:B:94:LEU:HG   | 7        | 0.42          |
| (1,1167) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HB2  | 4        | 0.42          |
| (1,1167) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HB3  | 4        | 0.42          |
| (1,115)  | 1:A:77:VAL:HG11 | 1:A:145:VAL:H   | 5        | 0.42          |
| (1,115)  | 1:A:77:VAL:HG12 | 1:A:145:VAL:H   | 5        | 0.42          |
| (1,115)  | 1:A:77:VAL:HG13 | 1:A:145:VAL:H   | 5        | 0.42          |
| (1,1111) | 1:B:89:LEU:HD21 | 1:B:88:GLU:H    | 2        | 0.42          |
| (1,1111) | 1:B:89:LEU:HD22 | 1:B:88:GLU:H    | 2        | 0.42          |
| (1,1111) | 1:B:89:LEU:HD23 | 1:B:88:GLU:H    | 2        | 0.42          |
| (1,1106) | 1:B:89:LEU:H    | 1:B:87:GLU:HA   | 8        | 0.42          |
| (1,1098) | 1:B:87:GLU:HB2  | 1:B:89:LEU:H    | 6        | 0.42          |
| (1,1098) | 1:B:87:GLU:HB3  | 1:B:89:LEU:H    | 6        | 0.42          |
| (1,1056) | 1:B:84:PHE:H    | 1:B:81:VAL:HB   | 1        | 0.42          |
| (1,955)  | 1:B:77:VAL:HG11 | 1:B:76:SER:HA   | 1        | 0.41          |
| (1,955)  | 1:B:77:VAL:HG12 | 1:B:76:SER:HA   | 1        | 0.41          |
| (1,955)  | 1:B:77:VAL:HG13 | 1:B:76:SER:HA   | 1        | 0.41          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,955) | 1:B:77:VAL:HG11  | 1:B:76:SER:HA    | 4        | 0.41          |
| (1,955) | 1:B:77:VAL:HG12  | 1:B:76:SER:HA    | 4        | 0.41          |
| (1,955) | 1:B:77:VAL:HG13  | 1:B:76:SER:HA    | 4        | 0.41          |
| (1,955) | 1:B:77:VAL:HG11  | 1:B:76:SER:HA    | 8        | 0.41          |
| (1,955) | 1:B:77:VAL:HG12  | 1:B:76:SER:HA    | 8        | 0.41          |
| (1,955) | 1:B:77:VAL:HG13  | 1:B:76:SER:HA    | 8        | 0.41          |
| (1,932) | 1:B:76:SER:HB2   | 1:B:144:THR:HG21 | 9        | 0.41          |
| (1,932) | 1:B:76:SER:HB2   | 1:B:144:THR:HG22 | 9        | 0.41          |
| (1,932) | 1:B:76:SER:HB2   | 1:B:144:THR:HG23 | 9        | 0.41          |
| (1,889) | 1:B:70:LEU:HB3   | 1:B:74:ARG:H     | 8        | 0.41          |
| (1,88)  | 1:A:77:VAL:HG11  | 1:A:76:SER:HA    | 1        | 0.41          |
| (1,88)  | 1:A:77:VAL:HG12  | 1:A:76:SER:HA    | 1        | 0.41          |
| (1,88)  | 1:A:77:VAL:HG13  | 1:A:76:SER:HA    | 1        | 0.41          |
| (1,88)  | 1:A:77:VAL:HG11  | 1:A:76:SER:HA    | 4        | 0.41          |
| (1,88)  | 1:A:77:VAL:HG12  | 1:A:76:SER:HA    | 4        | 0.41          |
| (1,88)  | 1:A:77:VAL:HG13  | 1:A:76:SER:HA    | 4        | 0.41          |
| (1,88)  | 1:A:77:VAL:HG11  | 1:A:76:SER:HA    | 8        | 0.41          |
| (1,88)  | 1:A:77:VAL:HG12  | 1:A:76:SER:HA    | 8        | 0.41          |
| (1,88)  | 1:A:77:VAL:HG13  | 1:A:76:SER:HA    | 8        | 0.41          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD11  | 9        | 0.41          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD12  | 9        | 0.41          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD13  | 9        | 0.41          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD21  | 9        | 0.41          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD22  | 9        | 0.41          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD23  | 9        | 0.41          |
| (1,783) | 1:A:142:VAL:HG11 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,783) | 1:A:142:VAL:HG12 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,783) | 1:A:142:VAL:HG13 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,783) | 1:A:142:VAL:HG21 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,783) | 1:A:142:VAL:HG22 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,783) | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,782) | 1:A:142:VAL:HG11 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,782) | 1:A:142:VAL:HG12 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,782) | 1:A:142:VAL:HG13 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,782) | 1:A:142:VAL:HG21 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,782) | 1:A:142:VAL:HG22 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,782) | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 3        | 0.41          |
| (1,724) | 1:A:133:ILE:HD11 | 1:A:134:THR:H    | 2        | 0.41          |
| (1,724) | 1:A:133:ILE:HD12 | 1:A:134:THR:H    | 2        | 0.41          |
| (1,724) | 1:A:133:ILE:HD13 | 1:A:134:THR:H    | 2        | 0.41          |
| (1,673) | 1:A:127:ASP:HB3  | 1:A:128:VAL:H    | 1        | 0.41          |
| (1,65)  | 1:A:76:SER:HB2   | 1:A:144:THR:HG21 | 9        | 0.41          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,65)  | 1:A:76:SER:HB2   | 1:A:144:THR:HG22 | 9        | 0.41          |
| (1,65)  | 1:A:76:SER:HB2   | 1:A:144:THR:HG23 | 9        | 0.41          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG12 | 9        | 0.41          |
| (1,629) | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG13 | 9        | 0.41          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG12 | 9        | 0.41          |
| (1,629) | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG13 | 9        | 0.41          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG12 | 9        | 0.41          |
| (1,629) | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG13 | 9        | 0.41          |
| (1,586) | 1:A:121:LYS:HA   | 1:A:122:TYR:H    | 4        | 0.41          |
| (1,585) | 1:A:121:LYS:HG2  | 1:A:121:LYS:HA   | 8        | 0.41          |
| (1,585) | 1:A:121:LYS:HG3  | 1:A:121:LYS:HA   | 8        | 0.41          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB2  | 1        | 0.41          |
| (1,584) | 1:A:121:LYS:HA   | 1:A:120:ARG:HB3  | 1        | 0.41          |
| (1,548) | 1:A:117:GLU:HA   | 1:A:118:PHE:H    | 7        | 0.41          |
| (1,540) | 1:A:116:ARG:HA   | 1:A:117:GLU:H    | 3        | 0.41          |
| (1,519) | 1:A:114:ILE:HB   | 1:A:114:ILE:H    | 4        | 0.41          |
| (1,445) | 1:A:108:GLN:HA   | 1:A:113:PHE:H    | 7        | 0.41          |
| (1,432) | 1:A:107:ARG:HG2  | 1:A:108:GLN:H    | 1        | 0.41          |
| (1,432) | 1:A:107:ARG:HG3  | 1:A:108:GLN:H    | 1        | 0.41          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD11  | 9        | 0.41          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD12  | 9        | 0.41          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD13  | 9        | 0.41          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD21  | 9        | 0.41          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD22  | 9        | 0.41          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD23  | 9        | 0.41          |
| (1,337) | 1:A:98:ILE:HD11  | 1:A:98:ILE:HB    | 9        | 0.41          |
| (1,337) | 1:A:98:ILE:HD12  | 1:A:98:ILE:HB    | 9        | 0.41          |
| (1,337) | 1:A:98:ILE:HD13  | 1:A:98:ILE:HB    | 9        | 0.41          |
| (1,332) | 1:A:97:VAL:HA    | 1:A:124:ILE:HG12 | 7        | 0.41          |
| (1,332) | 1:A:97:VAL:HA    | 1:A:124:ILE:HG13 | 7        | 0.41          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG11  | 6        | 0.41          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG12  | 6        | 0.41          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG13  | 6        | 0.41          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG21  | 6        | 0.41          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG22  | 6        | 0.41          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG23  | 6        | 0.41          |
| (1,301) | 1:A:95:GLY:H     | 1:A:94:LEU:HG    | 7        | 0.41          |
| (1,300) | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB2   | 7        | 0.41          |
| (1,300) | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB3   | 7        | 0.41          |
| (1,282) | 1:A:93:VAL:H     | 1:A:92:LYS:HG2   | 4        | 0.41          |
| (1,282) | 1:A:93:VAL:H     | 1:A:92:LYS:HG3   | 4        | 0.41          |
| (1,271) | 1:A:91:VAL:HB    | 1:A:92:LYS:H     | 8        | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD21  | 7        | 0.41          |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD22  | 7        | 0.41          |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD23  | 7        | 0.41          |
| (1,244)  | 1:A:89:LEU:HD21  | 1:A:88:GLU:H     | 2        | 0.41          |
| (1,244)  | 1:A:89:LEU:HD22  | 1:A:88:GLU:H     | 2        | 0.41          |
| (1,244)  | 1:A:89:LEU:HD23  | 1:A:88:GLU:H     | 2        | 0.41          |
| (1,218)  | 1:A:86:PRO:HB2   | 1:A:85:SER:HA    | 2        | 0.41          |
| (1,218)  | 1:A:86:PRO:HB3   | 1:A:85:SER:HA    | 2        | 0.41          |
| (1,218)  | 1:A:86:PRO:HB2   | 1:A:85:SER:HA    | 9        | 0.41          |
| (1,218)  | 1:A:86:PRO:HB3   | 1:A:85:SER:HA    | 9        | 0.41          |
| (1,198)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 2        | 0.41          |
| (1,198)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 2        | 0.41          |
| (1,196)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 2        | 0.41          |
| (1,196)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 2        | 0.41          |
| (1,184)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 6        | 0.41          |
| (1,183)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 6        | 0.41          |
| (1,1760) | 1:A:120:ARG:HB2  | 1:B:111:HIS:H    | 4        | 0.41          |
| (1,1760) | 1:A:120:ARG:HB3  | 1:B:111:HIS:H    | 4        | 0.41          |
| (1,1650) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,1650) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,1650) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,1650) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,1650) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,1650) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,1649) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,1649) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,1649) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,1649) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,1649) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,1649) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H    | 3        | 0.41          |
| (1,158)  | 1:A:81:VAL:H     | 1:A:81:VAL:HB    | 8        | 0.41          |
| (1,1540) | 1:B:127:ASP:HB3  | 1:B:128:VAL:H    | 1        | 0.41          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG12 | 9        | 0.41          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG13 | 9        | 0.41          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG12 | 9        | 0.41          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG13 | 9        | 0.41          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG12 | 9        | 0.41          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG13 | 9        | 0.41          |
| (1,1453) | 1:B:121:LYS:HA   | 1:B:122:TYR:H    | 4        | 0.41          |
| (1,1452) | 1:B:121:LYS:HG2  | 1:B:121:LYS:HA   | 8        | 0.41          |
| (1,1452) | 1:B:121:LYS:HG3  | 1:B:121:LYS:HA   | 8        | 0.41          |
| (1,1451) | 1:B:121:LYS:HA   | 1:B:120:ARG:HB2  | 1        | 0.41          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1451) | 1:B:121:LYS:HA  | 1:B:120:ARG:HB3  | 1        | 0.41          |
| (1,1415) | 1:B:117:GLU:HA  | 1:B:118:PHE:H    | 7        | 0.41          |
| (1,1407) | 1:B:116:ARG:HA  | 1:B:117:GLU:H    | 3        | 0.41          |
| (1,1386) | 1:B:114:ILE:HB  | 1:B:114:ILE:H    | 4        | 0.41          |
| (1,1332) | 1:B:111:HIS:HB2 | 1:B:111:HIS:H    | 6        | 0.41          |
| (1,1312) | 1:B:108:GLN:HA  | 1:B:113:PHE:H    | 7        | 0.41          |
| (1,1299) | 1:B:107:ARG:HG2 | 1:B:108:GLN:H    | 1        | 0.41          |
| (1,1299) | 1:B:107:ARG:HG3 | 1:B:108:GLN:H    | 1        | 0.41          |
| (1,1204) | 1:B:98:ILE:HD11 | 1:B:98:ILE:HB    | 3        | 0.41          |
| (1,1204) | 1:B:98:ILE:HD12 | 1:B:98:ILE:HB    | 3        | 0.41          |
| (1,1204) | 1:B:98:ILE:HD13 | 1:B:98:ILE:HB    | 3        | 0.41          |
| (1,1204) | 1:B:98:ILE:HD11 | 1:B:98:ILE:HB    | 9        | 0.41          |
| (1,1204) | 1:B:98:ILE:HD12 | 1:B:98:ILE:HB    | 9        | 0.41          |
| (1,1204) | 1:B:98:ILE:HD13 | 1:B:98:ILE:HB    | 9        | 0.41          |
| (1,1199) | 1:B:97:VAL:HA   | 1:B:124:ILE:HG12 | 7        | 0.41          |
| (1,1199) | 1:B:97:VAL:HA   | 1:B:124:ILE:HG13 | 7        | 0.41          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG11  | 6        | 0.41          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG12  | 6        | 0.41          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG13  | 6        | 0.41          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG21  | 6        | 0.41          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG22  | 6        | 0.41          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG23  | 6        | 0.41          |
| (1,1167) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HB2   | 7        | 0.41          |
| (1,1167) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HB3   | 7        | 0.41          |
| (1,1149) | 1:B:93:VAL:H    | 1:B:92:LYS:HG2   | 4        | 0.41          |
| (1,1149) | 1:B:93:VAL:H    | 1:B:92:LYS:HG3   | 4        | 0.41          |
| (1,1138) | 1:B:91:VAL:HB   | 1:B:92:LYS:H     | 8        | 0.41          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD21  | 7        | 0.41          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD22  | 7        | 0.41          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD23  | 7        | 0.41          |
| (1,1085) | 1:B:86:PRO:HB2  | 1:B:85:SER:HA    | 2        | 0.41          |
| (1,1085) | 1:B:86:PRO:HB3  | 1:B:85:SER:HA    | 2        | 0.41          |
| (1,1085) | 1:B:86:PRO:HB2  | 1:B:85:SER:HA    | 9        | 0.41          |
| (1,1085) | 1:B:86:PRO:HB3  | 1:B:85:SER:HA    | 9        | 0.41          |
| (1,107)  | 1:A:77:VAL:HG11 | 1:A:79:LEU:HG    | 5        | 0.41          |
| (1,107)  | 1:A:77:VAL:HG12 | 1:A:79:LEU:HG    | 5        | 0.41          |
| (1,107)  | 1:A:77:VAL:HG13 | 1:A:79:LEU:HG    | 5        | 0.41          |
| (1,1065) | 1:B:84:PHE:HB2  | 1:B:84:PHE:H     | 2        | 0.41          |
| (1,1065) | 1:B:84:PHE:HB3  | 1:B:84:PHE:H     | 2        | 0.41          |
| (1,1063) | 1:B:84:PHE:HB2  | 1:B:84:PHE:H     | 2        | 0.41          |
| (1,1063) | 1:B:84:PHE:HB3  | 1:B:84:PHE:H     | 2        | 0.41          |
| (1,1051) | 1:B:83:HIS:H    | 1:B:84:PHE:H     | 6        | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1050) | 1:B:83:HIS:H     | 1:B:84:PHE:H     | 6        | 0.41          |
| (1,1025) | 1:B:81:VAL:H     | 1:B:81:VAL:HB    | 8        | 0.41          |
| (1,980)  | 1:B:77:VAL:HB    | 1:B:145:VAL:HG21 | 6        | 0.4           |
| (1,980)  | 1:B:77:VAL:HB    | 1:B:145:VAL:HG22 | 6        | 0.4           |
| (1,980)  | 1:B:77:VAL:HB    | 1:B:145:VAL:HG23 | 6        | 0.4           |
| (1,929)  | 1:B:76:SER:HB3   | 1:B:76:SER:H     | 4        | 0.4           |
| (1,892)  | 1:B:71:GLU:H     | 1:B:71:GLU:HG2   | 8        | 0.4           |
| (1,892)  | 1:B:71:GLU:H     | 1:B:71:GLU:HG3   | 8        | 0.4           |
| (1,840)  | 1:A:146:ASP:HA   | 1:A:147:GLY:H    | 4        | 0.4           |
| (1,811)  | 1:A:145:VAL:HB   | 1:A:77:VAL:HB    | 8        | 0.4           |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD11 | 3        | 0.4           |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD12 | 3        | 0.4           |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD13 | 3        | 0.4           |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD21 | 3        | 0.4           |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD22 | 3        | 0.4           |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD23 | 3        | 0.4           |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB2  | 6        | 0.4           |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB3  | 6        | 0.4           |
| (1,633)  | 1:A:124:ILE:HA   | 1:A:124:ILE:H    | 4        | 0.4           |
| (1,629)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG12 | 5        | 0.4           |
| (1,629)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG13 | 5        | 0.4           |
| (1,629)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG12 | 5        | 0.4           |
| (1,629)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG13 | 5        | 0.4           |
| (1,629)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG12 | 5        | 0.4           |
| (1,629)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG13 | 5        | 0.4           |
| (1,621)  | 1:A:124:ILE:HD11 | 1:A:123:ARG:HA   | 5        | 0.4           |
| (1,621)  | 1:A:124:ILE:HD12 | 1:A:123:ARG:HA   | 5        | 0.4           |
| (1,621)  | 1:A:124:ILE:HD13 | 1:A:123:ARG:HA   | 5        | 0.4           |
| (1,62)   | 1:A:76:SER:HB3   | 1:A:76:SER:H     | 4        | 0.4           |
| (1,574)  | 1:A:119:HIS:HB3  | 1:A:119:HIS:HD2  | 2        | 0.4           |
| (1,573)  | 1:A:119:HIS:HA   | 1:A:119:HIS:HD2  | 7        | 0.4           |
| (1,539)  | 1:A:116:ARG:H    | 1:A:116:ARG:HG2  | 8        | 0.4           |
| (1,539)  | 1:A:116:ARG:H    | 1:A:116:ARG:HG3  | 8        | 0.4           |
| (1,524)  | 1:A:115:SER:HB2  | 1:A:106:GLU:H    | 2        | 0.4           |
| (1,491)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 8        | 0.4           |
| (1,489)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 8        | 0.4           |
| (1,465)  | 1:A:111:HIS:HB2  | 1:A:111:HIS:H    | 6        | 0.4           |
| (1,46)   | 1:A:75:PHE:HA    | 1:A:75:PHE:HB2   | 9        | 0.4           |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG2   | 2        | 0.4           |
| (1,393)  | 1:A:103:LYS:H    | 1:A:88:GLU:HG3   | 2        | 0.4           |
| (1,354)  | 1:A:99:GLU:HA    | 1:A:100:VAL:H    | 7        | 0.4           |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG21 | 8        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG22 | 8        | 0.4           |
| (1,352)  | 1:A:99:GLU:HB2   | 1:A:100:VAL:HG23 | 8        | 0.4           |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG21 | 8        | 0.4           |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG22 | 8        | 0.4           |
| (1,352)  | 1:A:99:GLU:HB3   | 1:A:100:VAL:HG23 | 8        | 0.4           |
| (1,337)  | 1:A:98:ILE:HD11  | 1:A:98:ILE:HB    | 3        | 0.4           |
| (1,337)  | 1:A:98:ILE:HD12  | 1:A:98:ILE:HB    | 3        | 0.4           |
| (1,337)  | 1:A:98:ILE:HD13  | 1:A:98:ILE:HB    | 3        | 0.4           |
| (1,323)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HB2   | 2        | 0.4           |
| (1,323)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HB3   | 2        | 0.4           |
| (1,306)  | 1:A:95:GLY:HA2   | 1:A:97:VAL:H     | 3        | 0.4           |
| (1,287)  | 1:A:93:VAL:HA    | 1:A:98:ILE:HA    | 4        | 0.4           |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG2   | 8        | 0.4           |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG3   | 8        | 0.4           |
| (1,239)  | 1:A:89:LEU:H     | 1:A:87:GLU:HA    | 1        | 0.4           |
| (1,218)  | 1:A:86:PRO:HB2   | 1:A:85:SER:HA    | 8        | 0.4           |
| (1,218)  | 1:A:86:PRO:HB3   | 1:A:85:SER:HA    | 8        | 0.4           |
| (1,216)  | 1:A:85:SER:HB2   | 1:A:89:LEU:H     | 3        | 0.4           |
| (1,215)  | 1:A:85:SER:HB3   | 1:A:89:LEU:H     | 3        | 0.4           |
| (1,199)  | 1:A:84:PHE:HB2   | 1:A:85:SER:H     | 7        | 0.4           |
| (1,199)  | 1:A:84:PHE:HB3   | 1:A:85:SER:H     | 7        | 0.4           |
| (1,184)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 8        | 0.4           |
| (1,183)  | 1:A:83:HIS:H     | 1:A:84:PHE:H     | 8        | 0.4           |
| (1,1770) | 1:A:123:ARG:HD2  | 1:B:113:PHE:H    | 7        | 0.4           |
| (1,1770) | 1:A:123:ARG:HD3  | 1:B:113:PHE:H    | 7        | 0.4           |
| (1,1751) | 1:A:118:PHE:HD1  | 1:B:114:ILE:HG21 | 5        | 0.4           |
| (1,1751) | 1:A:118:PHE:HD1  | 1:B:114:ILE:HG22 | 5        | 0.4           |
| (1,1751) | 1:A:118:PHE:HD1  | 1:B:114:ILE:HG23 | 5        | 0.4           |
| (1,1751) | 1:A:118:PHE:HD2  | 1:B:114:ILE:HG21 | 5        | 0.4           |
| (1,1751) | 1:A:118:PHE:HD2  | 1:B:114:ILE:HG22 | 5        | 0.4           |
| (1,1751) | 1:A:118:PHE:HD2  | 1:B:114:ILE:HG23 | 5        | 0.4           |
| (1,1707) | 1:B:146:ASP:HA   | 1:B:147:GLY:H    | 4        | 0.4           |
| (1,1678) | 1:B:145:VAL:HB   | 1:B:77:VAL:HB    | 8        | 0.4           |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD11 | 3        | 0.4           |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD12 | 3        | 0.4           |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD13 | 3        | 0.4           |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD21 | 3        | 0.4           |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD22 | 3        | 0.4           |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD23 | 3        | 0.4           |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB2  | 6        | 0.4           |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB3  | 6        | 0.4           |
| (1,1502) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 4        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1502) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 4        | 0.4           |
| (1,1502) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H    | 4        | 0.4           |
| (1,1501) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 4        | 0.4           |
| (1,1501) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 4        | 0.4           |
| (1,1501) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H    | 4        | 0.4           |
| (1,1500) | 1:B:124:ILE:HA   | 1:B:124:ILE:H    | 4        | 0.4           |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG12 | 5        | 0.4           |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG13 | 5        | 0.4           |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG12 | 5        | 0.4           |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG13 | 5        | 0.4           |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG12 | 5        | 0.4           |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG13 | 5        | 0.4           |
| (1,1488) | 1:B:124:ILE:HD11 | 1:B:123:ARG:HA   | 5        | 0.4           |
| (1,1488) | 1:B:124:ILE:HD12 | 1:B:123:ARG:HA   | 5        | 0.4           |
| (1,1488) | 1:B:124:ILE:HD13 | 1:B:123:ARG:HA   | 5        | 0.4           |
| (1,1441) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HD2  | 2        | 0.4           |
| (1,1441) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HD2  | 5        | 0.4           |
| (1,1440) | 1:B:119:HIS:HA   | 1:B:119:HIS:HD2  | 7        | 0.4           |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG2  | 8        | 0.4           |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG3  | 8        | 0.4           |
| (1,1358) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3  | 8        | 0.4           |
| (1,1356) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3  | 8        | 0.4           |
| (1,1250) | 1:B:101:HIS:HA   | 1:B:119:HIS:HD2  | 3        | 0.4           |
| (1,1221) | 1:B:99:GLU:HA    | 1:B:100:VAL:H    | 7        | 0.4           |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG21 | 8        | 0.4           |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG22 | 8        | 0.4           |
| (1,1219) | 1:B:99:GLU:HB2   | 1:B:100:VAL:HG23 | 8        | 0.4           |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG21 | 8        | 0.4           |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG22 | 8        | 0.4           |
| (1,1219) | 1:B:99:GLU:HB3   | 1:B:100:VAL:HG23 | 8        | 0.4           |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB2   | 2        | 0.4           |
| (1,1190) | 1:B:97:VAL:HB    | 1:B:94:LEU:HB3   | 2        | 0.4           |
| (1,1173) | 1:B:95:GLY:HA2   | 1:B:97:VAL:H     | 3        | 0.4           |
| (1,1154) | 1:B:93:VAL:HA    | 1:B:98:ILE:HA    | 4        | 0.4           |
| (1,113)  | 1:A:77:VAL:HB    | 1:A:145:VAL:HG21 | 6        | 0.4           |
| (1,113)  | 1:A:77:VAL:HB    | 1:A:145:VAL:HG22 | 6        | 0.4           |
| (1,113)  | 1:A:77:VAL:HB    | 1:A:145:VAL:HG23 | 6        | 0.4           |
| (1,1106) | 1:B:89:LEU:H     | 1:B:87:GLU:HA    | 1        | 0.4           |
| (1,1085) | 1:B:86:PRO:HB2   | 1:B:85:SER:HA    | 8        | 0.4           |
| (1,1085) | 1:B:86:PRO:HB3   | 1:B:85:SER:HA    | 8        | 0.4           |
| (1,1083) | 1:B:85:SER:HB2   | 1:B:89:LEU:H     | 3        | 0.4           |
| (1,1082) | 1:B:85:SER:HB3   | 1:B:89:LEU:H     | 3        | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1066) | 1:B:84:PHE:HB2   | 1:B:85:SER:H     | 7        | 0.4           |
| (1,1066) | 1:B:84:PHE:HB3   | 1:B:85:SER:H     | 7        | 0.4           |
| (1,1051) | 1:B:83:HIS:H     | 1:B:84:PHE:H     | 8        | 0.4           |
| (1,1050) | 1:B:83:HIS:H     | 1:B:84:PHE:H     | 8        | 0.4           |
| (1,1040) | 1:B:83:HIS:HA    | 1:B:83:HIS:HD2   | 9        | 0.4           |
| (1,986)  | 1:B:77:VAL:HB    | 1:B:146:ASP:HB3  | 7        | 0.39          |
| (1,913)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HB2   | 9        | 0.39          |
| (1,897)  | 1:B:72:LYS:H     | 1:B:72:LYS:HG2   | 3        | 0.39          |
| (1,897)  | 1:B:72:LYS:H     | 1:B:72:LYS:HG3   | 3        | 0.39          |
| (1,889)  | 1:B:70:LEU:HB3   | 1:B:74:ARG:H     | 2        | 0.39          |
| (1,848)  | 1:A:147:GLY:HA3  | 1:A:147:GLY:H    | 2        | 0.39          |
| (1,708)  | 1:A:132:THR:H    | 1:A:133:ILE:H    | 6        | 0.39          |
| (1,706)  | 1:A:132:THR:H    | 1:A:133:ILE:H    | 6        | 0.39          |
| (1,680)  | 1:A:128:VAL:H    | 1:A:129:ASP:H    | 4        | 0.39          |
| (1,673)  | 1:A:127:ASP:HB3  | 1:A:128:VAL:H    | 9        | 0.39          |
| (1,647)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD11 | 4        | 0.39          |
| (1,647)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD12 | 4        | 0.39          |
| (1,647)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD13 | 4        | 0.39          |
| (1,647)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD11 | 5        | 0.39          |
| (1,647)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD12 | 5        | 0.39          |
| (1,647)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD13 | 5        | 0.39          |
| (1,635)  | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 4        | 0.39          |
| (1,635)  | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 4        | 0.39          |
| (1,635)  | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 4        | 0.39          |
| (1,634)  | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 4        | 0.39          |
| (1,634)  | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 4        | 0.39          |
| (1,634)  | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 4        | 0.39          |
| (1,629)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG12 | 2        | 0.39          |
| (1,629)  | 1:A:124:ILE:HG21 | 1:A:124:ILE:HG13 | 2        | 0.39          |
| (1,629)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG12 | 2        | 0.39          |
| (1,629)  | 1:A:124:ILE:HG22 | 1:A:124:ILE:HG13 | 2        | 0.39          |
| (1,629)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG12 | 2        | 0.39          |
| (1,629)  | 1:A:124:ILE:HG23 | 1:A:124:ILE:HG13 | 2        | 0.39          |
| (1,615)  | 1:A:124:ILE:HB   | 1:A:97:VAL:HA    | 9        | 0.39          |
| (1,585)  | 1:A:121:LYS:HG2  | 1:A:121:LYS:HA   | 1        | 0.39          |
| (1,585)  | 1:A:121:LYS:HG3  | 1:A:121:LYS:HA   | 1        | 0.39          |
| (1,585)  | 1:A:121:LYS:HG2  | 1:A:121:LYS:HA   | 2        | 0.39          |
| (1,585)  | 1:A:121:LYS:HG3  | 1:A:121:LYS:HA   | 2        | 0.39          |
| (1,578)  | 1:A:119:HIS:HA   | 1:A:119:HIS:H    | 2        | 0.39          |
| (1,578)  | 1:A:119:HIS:HA   | 1:A:119:HIS:H    | 8        | 0.39          |
| (1,552)  | 1:A:118:PHE:HE1  | 1:A:103:LYS:H    | 6        | 0.39          |
| (1,552)  | 1:A:118:PHE:HE2  | 1:A:103:LYS:H    | 6        | 0.39          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,535)  | 1:A:116:ARG:H    | 1:A:104:HIS:H   | 1        | 0.39          |
| (1,534)  | 1:A:116:ARG:H    | 1:A:104:HIS:H   | 1        | 0.39          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB2 | 8        | 0.39          |
| (1,503)  | 1:A:114:ILE:HD11 | 1:A:106:GLU:HB3 | 8        | 0.39          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB2 | 8        | 0.39          |
| (1,503)  | 1:A:114:ILE:HD12 | 1:A:106:GLU:HB3 | 8        | 0.39          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB2 | 8        | 0.39          |
| (1,503)  | 1:A:114:ILE:HD13 | 1:A:106:GLU:HB3 | 8        | 0.39          |
| (1,497)  | 1:A:113:PHE:HD1  | 1:A:113:PHE:H   | 6        | 0.39          |
| (1,497)  | 1:A:113:PHE:HD2  | 1:A:113:PHE:H   | 6        | 0.39          |
| (1,494)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HD1 | 3        | 0.39          |
| (1,494)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HD2 | 3        | 0.39          |
| (1,491)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3 | 3        | 0.39          |
| (1,489)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3 | 3        | 0.39          |
| (1,468)  | 1:A:111:HIS:H    | 1:A:112:GLY:H   | 2        | 0.39          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB2 | 6        | 0.39          |
| (1,453)  | 1:A:110:GLU:H    | 1:A:109:ASP:HB3 | 6        | 0.39          |
| (1,432)  | 1:A:107:ARG:HG2  | 1:A:108:GLN:H   | 6        | 0.39          |
| (1,432)  | 1:A:107:ARG:HG3  | 1:A:108:GLN:H   | 6        | 0.39          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD2 | 1        | 0.39          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD3 | 1        | 0.39          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD2 | 3        | 0.39          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD3 | 3        | 0.39          |
| (1,379)  | 1:A:101:HIS:HB2  | 1:A:101:HIS:H   | 9        | 0.39          |
| (1,354)  | 1:A:99:GLU:HA    | 1:A:100:VAL:H   | 5        | 0.39          |
| (1,300)  | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB2  | 9        | 0.39          |
| (1,300)  | 1:A:95:GLY:HA3   | 1:A:94:LEU:HB3  | 9        | 0.39          |
| (1,30)   | 1:A:72:LYS:H     | 1:A:72:LYS:HG2  | 3        | 0.39          |
| (1,30)   | 1:A:72:LYS:H     | 1:A:72:LYS:HG3  | 3        | 0.39          |
| (1,279)  | 1:A:92:LYS:H     | 1:A:99:GLU:H    | 9        | 0.39          |
| (1,239)  | 1:A:89:LEU:H     | 1:A:87:GLU:HA   | 6        | 0.39          |
| (1,22)   | 1:A:70:LEU:HB3   | 1:A:74:ARG:H    | 2        | 0.39          |
| (1,218)  | 1:A:86:PRO:HB2   | 1:A:85:SER:HA   | 6        | 0.39          |
| (1,218)  | 1:A:86:PRO:HB3   | 1:A:85:SER:HA   | 6        | 0.39          |
| (1,1762) | 1:A:122:TYR:HB2  | 1:B:111:HIS:H   | 8        | 0.39          |
| (1,1762) | 1:A:122:TYR:HB3  | 1:B:111:HIS:H   | 8        | 0.39          |
| (1,1715) | 1:B:147:GLY:HA3  | 1:B:147:GLY:H   | 2        | 0.39          |
| (1,1637) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 3        | 0.39          |
| (1,1635) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 3        | 0.39          |
| (1,1591) | 1:B:133:ILE:HD11 | 1:B:134:THR:H   | 2        | 0.39          |
| (1,1591) | 1:B:133:ILE:HD12 | 1:B:134:THR:H   | 2        | 0.39          |
| (1,1591) | 1:B:133:ILE:HD13 | 1:B:134:THR:H   | 2        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1586) | 1:B:133:ILE:HG21 | 1:B:133:ILE:HA   | 2        | 0.39          |
| (1,1586) | 1:B:133:ILE:HG22 | 1:B:133:ILE:HA   | 2        | 0.39          |
| (1,1586) | 1:B:133:ILE:HG23 | 1:B:133:ILE:HA   | 2        | 0.39          |
| (1,1575) | 1:B:132:THR:H    | 1:B:133:ILE:H    | 6        | 0.39          |
| (1,1573) | 1:B:132:THR:H    | 1:B:133:ILE:H    | 6        | 0.39          |
| (1,1540) | 1:B:127:ASP:HB3  | 1:B:128:VAL:H    | 9        | 0.39          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD11 | 4        | 0.39          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD12 | 4        | 0.39          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD13 | 4        | 0.39          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG12 | 2        | 0.39          |
| (1,1496) | 1:B:124:ILE:HG21 | 1:B:124:ILE:HG13 | 2        | 0.39          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG12 | 2        | 0.39          |
| (1,1496) | 1:B:124:ILE:HG22 | 1:B:124:ILE:HG13 | 2        | 0.39          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG12 | 2        | 0.39          |
| (1,1496) | 1:B:124:ILE:HG23 | 1:B:124:ILE:HG13 | 2        | 0.39          |
| (1,1482) | 1:B:124:ILE:HB   | 1:B:97:VAL:HA    | 9        | 0.39          |
| (1,1452) | 1:B:121:LYS:HG2  | 1:B:121:LYS:HA   | 1        | 0.39          |
| (1,1452) | 1:B:121:LYS:HG3  | 1:B:121:LYS:HA   | 1        | 0.39          |
| (1,1452) | 1:B:121:LYS:HG2  | 1:B:121:LYS:HA   | 2        | 0.39          |
| (1,1452) | 1:B:121:LYS:HG3  | 1:B:121:LYS:HA   | 2        | 0.39          |
| (1,1445) | 1:B:119:HIS:HA   | 1:B:119:HIS:H    | 2        | 0.39          |
| (1,1445) | 1:B:119:HIS:HA   | 1:B:119:HIS:H    | 8        | 0.39          |
| (1,1441) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HD2  | 3        | 0.39          |
| (1,1419) | 1:B:118:PHE:HE1  | 1:B:103:LYS:H    | 6        | 0.39          |
| (1,1419) | 1:B:118:PHE:HE2  | 1:B:103:LYS:H    | 6        | 0.39          |
| (1,1402) | 1:B:116:ARG:H    | 1:B:104:HIS:H    | 1        | 0.39          |
| (1,1401) | 1:B:116:ARG:H    | 1:B:104:HIS:H    | 1        | 0.39          |
| (1,1391) | 1:B:115:SER:HB2  | 1:B:106:GLU:H    | 2        | 0.39          |
| (1,1364) | 1:B:113:PHE:HD1  | 1:B:113:PHE:H    | 6        | 0.39          |
| (1,1364) | 1:B:113:PHE:HD2  | 1:B:113:PHE:H    | 6        | 0.39          |
| (1,1361) | 1:B:113:PHE:HA   | 1:B:113:PHE:HD1  | 3        | 0.39          |
| (1,1361) | 1:B:113:PHE:HA   | 1:B:113:PHE:HD2  | 3        | 0.39          |
| (1,1335) | 1:B:111:HIS:H    | 1:B:112:GLY:H    | 2        | 0.39          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB2  | 6        | 0.39          |
| (1,1320) | 1:B:110:GLU:H    | 1:B:109:ASP:HB3  | 6        | 0.39          |
| (1,1299) | 1:B:107:ARG:HG2  | 1:B:108:GLN:H    | 6        | 0.39          |
| (1,1299) | 1:B:107:ARG:HG3  | 1:B:108:GLN:H    | 6        | 0.39          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD2  | 1        | 0.39          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD3  | 1        | 0.39          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD2  | 3        | 0.39          |
| (1,1261) | 1:B:103:LYS:HA   | 1:B:103:LYS:HD3  | 3        | 0.39          |
| (1,1260) | 1:B:103:LYS:H    | 1:B:88:GLU:HG2   | 2        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1260) | 1:B:103:LYS:H    | 1:B:88:GLU:HG3   | 2        | 0.39          |
| (1,1246) | 1:B:101:HIS:HB2  | 1:B:101:HIS:H    | 9        | 0.39          |
| (1,1221) | 1:B:99:GLU:HA    | 1:B:100:VAL:H    | 5        | 0.39          |
| (1,119)  | 1:A:77:VAL:HB    | 1:A:146:ASP:HB3  | 7        | 0.39          |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB2   | 9        | 0.39          |
| (1,1167) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HB3   | 9        | 0.39          |
| (1,1146) | 1:B:92:LYS:H     | 1:B:99:GLU:H     | 9        | 0.39          |
| (1,1106) | 1:B:89:LEU:H     | 1:B:87:GLU:HA    | 6        | 0.39          |
| (1,1085) | 1:B:86:PRO:HB2   | 1:B:85:SER:HA    | 6        | 0.39          |
| (1,1085) | 1:B:86:PRO:HB3   | 1:B:85:SER:HA    | 6        | 0.39          |
| (1,972)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HG    | 3        | 0.38          |
| (1,972)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HG    | 3        | 0.38          |
| (1,972)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HG    | 3        | 0.38          |
| (1,930)  | 1:B:76:SER:HB2   | 1:B:77:VAL:H     | 5        | 0.38          |
| (1,929)  | 1:B:76:SER:HB3   | 1:B:76:SER:H     | 3        | 0.38          |
| (1,913)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HB2   | 1        | 0.38          |
| (1,913)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HB2   | 3        | 0.38          |
| (1,913)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HB2   | 4        | 0.38          |
| (1,913)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HB2   | 5        | 0.38          |
| (1,866)  | 1:A:152:VAL:H    | 1:A:151:GLN:H    | 6        | 0.38          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD11 | 2        | 0.38          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD12 | 2        | 0.38          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD13 | 2        | 0.38          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD21 | 2        | 0.38          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD22 | 2        | 0.38          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD23 | 2        | 0.38          |
| (1,770)  | 1:A:141:GLY:H    | 1:A:140:ASP:H    | 3        | 0.38          |
| (1,768)  | 1:A:141:GLY:H    | 1:A:140:ASP:H    | 3        | 0.38          |
| (1,719)  | 1:A:133:ILE:HG21 | 1:A:133:ILE:HA   | 2        | 0.38          |
| (1,719)  | 1:A:133:ILE:HG22 | 1:A:133:ILE:HA   | 2        | 0.38          |
| (1,719)  | 1:A:133:ILE:HG23 | 1:A:133:ILE:HA   | 2        | 0.38          |
| (1,717)  | 1:A:133:ILE:HG21 | 1:A:132:THR:H    | 4        | 0.38          |
| (1,717)  | 1:A:133:ILE:HG22 | 1:A:132:THR:H    | 4        | 0.38          |
| (1,717)  | 1:A:133:ILE:HG23 | 1:A:132:THR:H    | 4        | 0.38          |
| (1,681)  | 1:A:128:VAL:H    | 1:A:150:LYS:HD2  | 1        | 0.38          |
| (1,681)  | 1:A:128:VAL:H    | 1:A:150:LYS:HD3  | 1        | 0.38          |
| (1,673)  | 1:A:127:ASP:HB3  | 1:A:128:VAL:H    | 2        | 0.38          |
| (1,63)   | 1:A:76:SER:HB2   | 1:A:77:VAL:H     | 5        | 0.38          |
| (1,62)   | 1:A:76:SER:HB3   | 1:A:76:SER:H     | 3        | 0.38          |
| (1,586)  | 1:A:121:LYS:HA   | 1:A:122:TYR:H    | 3        | 0.38          |
| (1,586)  | 1:A:121:LYS:HA   | 1:A:122:TYR:H    | 9        | 0.38          |
| (1,578)  | 1:A:119:HIS:HA   | 1:A:119:HIS:H    | 3        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,574)  | 1:A:119:HIS:HB3  | 1:A:119:HIS:HD2  | 1        | 0.38          |
| (1,574)  | 1:A:119:HIS:HB3  | 1:A:119:HIS:HD2  | 6        | 0.38          |
| (1,491)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 6        | 0.38          |
| (1,489)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 6        | 0.38          |
| (1,468)  | 1:A:111:HIS:H    | 1:A:112:GLY:H    | 4        | 0.38          |
| (1,46)   | 1:A:75:PHE:HA    | 1:A:75:PHE:HB2   | 1        | 0.38          |
| (1,46)   | 1:A:75:PHE:HA    | 1:A:75:PHE:HB2   | 3        | 0.38          |
| (1,46)   | 1:A:75:PHE:HA    | 1:A:75:PHE:HB2   | 4        | 0.38          |
| (1,46)   | 1:A:75:PHE:HA    | 1:A:75:PHE:HB2   | 5        | 0.38          |
| (1,445)  | 1:A:108:GLN:HA   | 1:A:113:PHE:H    | 8        | 0.38          |
| (1,437)  | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD1  | 5        | 0.38          |
| (1,437)  | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD2  | 5        | 0.38          |
| (1,434)  | 1:A:107:ARG:HD3  | 1:A:109:ASP:H    | 3        | 0.38          |
| (1,432)  | 1:A:107:ARG:HG2  | 1:A:108:GLN:H    | 8        | 0.38          |
| (1,432)  | 1:A:107:ARG:HG3  | 1:A:108:GLN:H    | 8        | 0.38          |
| (1,395)  | 1:A:103:LYS:HG2  | 1:A:103:LYS:H    | 5        | 0.38          |
| (1,395)  | 1:A:103:LYS:HG3  | 1:A:103:LYS:H    | 5        | 0.38          |
| (1,378)  | 1:A:101:HIS:HB3  | 1:A:101:HIS:H    | 1        | 0.38          |
| (1,378)  | 1:A:101:HIS:HB3  | 1:A:101:HIS:H    | 6        | 0.38          |
| (1,323)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HB2   | 8        | 0.38          |
| (1,323)  | 1:A:97:VAL:HB    | 1:A:94:LEU:HB3   | 8        | 0.38          |
| (1,309)  | 1:A:96:ASP:H     | 1:A:95:GLY:H     | 3        | 0.38          |
| (1,306)  | 1:A:95:GLY:HA2   | 1:A:97:VAL:H     | 5        | 0.38          |
| (1,289)  | 1:A:94:LEU:H     | 1:A:93:VAL:HB    | 8        | 0.38          |
| (1,1739) | 1:A:111:HIS:HA   | 1:B:122:TYR:HE1  | 6        | 0.38          |
| (1,1739) | 1:A:111:HIS:HA   | 1:B:122:TYR:HE2  | 6        | 0.38          |
| (1,1733) | 1:B:152:VAL:H    | 1:B:151:GLN:H    | 6        | 0.38          |
| (1,167)  | 1:A:81:VAL:H     | 1:A:141:GLY:HA2  | 4        | 0.38          |
| (1,1584) | 1:B:133:ILE:HG21 | 1:B:132:THR:H    | 4        | 0.38          |
| (1,1584) | 1:B:133:ILE:HG22 | 1:B:132:THR:H    | 4        | 0.38          |
| (1,1584) | 1:B:133:ILE:HG23 | 1:B:132:THR:H    | 4        | 0.38          |
| (1,155)  | 1:A:81:VAL:HG11  | 1:A:81:VAL:HA    | 7        | 0.38          |
| (1,155)  | 1:A:81:VAL:HG12  | 1:A:81:VAL:HA    | 7        | 0.38          |
| (1,155)  | 1:A:81:VAL:HG13  | 1:A:81:VAL:HA    | 7        | 0.38          |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD2  | 1        | 0.38          |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD3  | 1        | 0.38          |
| (1,1547) | 1:B:128:VAL:H    | 1:B:129:ASP:H    | 4        | 0.38          |
| (1,1540) | 1:B:127:ASP:HB3  | 1:B:128:VAL:H    | 2        | 0.38          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD11 | 5        | 0.38          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD12 | 5        | 0.38          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD13 | 5        | 0.38          |
| (1,1453) | 1:B:121:LYS:HA   | 1:B:122:TYR:H    | 3        | 0.38          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1453) | 1:B:121:LYS:HA  | 1:B:122:TYR:H   | 9        | 0.38          |
| (1,1445) | 1:B:119:HIS:HA  | 1:B:119:HIS:H   | 3        | 0.38          |
| (1,1358) | 1:B:113:PHE:HA  | 1:B:113:PHE:HB3 | 3        | 0.38          |
| (1,1358) | 1:B:113:PHE:HA  | 1:B:113:PHE:HB3 | 6        | 0.38          |
| (1,1356) | 1:B:113:PHE:HA  | 1:B:113:PHE:HB3 | 3        | 0.38          |
| (1,1356) | 1:B:113:PHE:HA  | 1:B:113:PHE:HB3 | 6        | 0.38          |
| (1,1335) | 1:B:111:HIS:H   | 1:B:112:GLY:H   | 4        | 0.38          |
| (1,1312) | 1:B:108:GLN:HA  | 1:B:113:PHE:H   | 8        | 0.38          |
| (1,1301) | 1:B:107:ARG:HD3 | 1:B:109:ASP:H   | 3        | 0.38          |
| (1,1299) | 1:B:107:ARG:HG2 | 1:B:108:GLN:H   | 8        | 0.38          |
| (1,1299) | 1:B:107:ARG:HG3 | 1:B:108:GLN:H   | 8        | 0.38          |
| (1,1262) | 1:B:103:LYS:HG2 | 1:B:103:LYS:H   | 5        | 0.38          |
| (1,1262) | 1:B:103:LYS:HG3 | 1:B:103:LYS:H   | 5        | 0.38          |
| (1,1245) | 1:B:101:HIS:HB3 | 1:B:101:HIS:H   | 1        | 0.38          |
| (1,1190) | 1:B:97:VAL:HB   | 1:B:94:LEU:HB2  | 8        | 0.38          |
| (1,1190) | 1:B:97:VAL:HB   | 1:B:94:LEU:HB3  | 8        | 0.38          |
| (1,1176) | 1:B:96:ASP:H    | 1:B:95:GLY:H    | 3        | 0.38          |
| (1,1173) | 1:B:95:GLY:HA2  | 1:B:97:VAL:H    | 5        | 0.38          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD11 | 4        | 0.38          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD12 | 4        | 0.38          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD13 | 4        | 0.38          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD21 | 4        | 0.38          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD22 | 4        | 0.38          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD23 | 4        | 0.38          |
| (1,105)  | 1:A:77:VAL:HG21 | 1:A:79:LEU:HG   | 3        | 0.38          |
| (1,105)  | 1:A:77:VAL:HG22 | 1:A:79:LEU:HG   | 3        | 0.38          |
| (1,105)  | 1:A:77:VAL:HG23 | 1:A:79:LEU:HG   | 3        | 0.38          |
| (1,1034) | 1:B:81:VAL:H    | 1:B:141:GLY:HA2 | 4        | 0.38          |
| (1,1022) | 1:B:81:VAL:HG11 | 1:B:81:VAL:HA   | 7        | 0.38          |
| (1,1022) | 1:B:81:VAL:HG12 | 1:B:81:VAL:HA   | 7        | 0.38          |
| (1,1022) | 1:B:81:VAL:HG13 | 1:B:81:VAL:HA   | 7        | 0.38          |
| (1,985)  | 1:B:77:VAL:HB   | 1:B:146:ASP:HB2 | 1        | 0.37          |
| (1,97)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:H    | 2        | 0.37          |
| (1,97)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:H    | 2        | 0.37          |
| (1,97)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:H    | 2        | 0.37          |
| (1,964)  | 1:B:77:VAL:HG21 | 1:B:77:VAL:H    | 2        | 0.37          |
| (1,964)  | 1:B:77:VAL:HG22 | 1:B:77:VAL:H    | 2        | 0.37          |
| (1,964)  | 1:B:77:VAL:HG23 | 1:B:77:VAL:H    | 2        | 0.37          |
| (1,955)  | 1:B:77:VAL:HG11 | 1:B:76:SER:HA   | 3        | 0.37          |
| (1,955)  | 1:B:77:VAL:HG12 | 1:B:76:SER:HA   | 3        | 0.37          |
| (1,955)  | 1:B:77:VAL:HG13 | 1:B:76:SER:HA   | 3        | 0.37          |
| (1,913)  | 1:B:75:PHE:HA   | 1:B:75:PHE:HB2  | 7        | 0.37          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,881) | 1:B:68:MET:HE1   | 1:B:122:TYR:HD1  | 2        | 0.37          |
| (1,881) | 1:B:68:MET:HE1   | 1:B:122:TYR:HD2  | 2        | 0.37          |
| (1,881) | 1:B:68:MET:HE2   | 1:B:122:TYR:HD1  | 2        | 0.37          |
| (1,881) | 1:B:68:MET:HE2   | 1:B:122:TYR:HD2  | 2        | 0.37          |
| (1,881) | 1:B:68:MET:HE3   | 1:B:122:TYR:HD1  | 2        | 0.37          |
| (1,881) | 1:B:68:MET:HE3   | 1:B:122:TYR:HD2  | 2        | 0.37          |
| (1,88)  | 1:A:77:VAL:HG11  | 1:A:76:SER:HA    | 3        | 0.37          |
| (1,88)  | 1:A:77:VAL:HG12  | 1:A:76:SER:HA    | 3        | 0.37          |
| (1,88)  | 1:A:77:VAL:HG13  | 1:A:76:SER:HA    | 3        | 0.37          |
| (1,879) | 1:B:68:MET:HE1   | 1:B:70:LEU:HD11  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE1   | 1:B:70:LEU:HD12  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE1   | 1:B:70:LEU:HD13  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE1   | 1:B:70:LEU:HD21  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE1   | 1:B:70:LEU:HD22  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE1   | 1:B:70:LEU:HD23  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE2   | 1:B:70:LEU:HD11  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE2   | 1:B:70:LEU:HD12  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE2   | 1:B:70:LEU:HD13  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE2   | 1:B:70:LEU:HD21  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE2   | 1:B:70:LEU:HD22  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE2   | 1:B:70:LEU:HD23  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE3   | 1:B:70:LEU:HD11  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE3   | 1:B:70:LEU:HD12  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE3   | 1:B:70:LEU:HD13  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE3   | 1:B:70:LEU:HD21  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE3   | 1:B:70:LEU:HD22  | 4        | 0.37          |
| (1,879) | 1:B:68:MET:HE3   | 1:B:70:LEU:HD23  | 4        | 0.37          |
| (1,804) | 1:A:144:THR:HA   | 1:A:145:VAL:H    | 3        | 0.37          |
| (1,804) | 1:A:144:THR:HA   | 1:A:145:VAL:H    | 4        | 0.37          |
| (1,804) | 1:A:144:THR:HA   | 1:A:145:VAL:H    | 7        | 0.37          |
| (1,744) | 1:A:135:SER:HB3  | 1:A:146:ASP:H    | 4        | 0.37          |
| (1,673) | 1:A:127:ASP:HB3  | 1:A:128:VAL:H    | 3        | 0.37          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD11 | 2        | 0.37          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD12 | 2        | 0.37          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD13 | 2        | 0.37          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD11 | 9        | 0.37          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD12 | 9        | 0.37          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD13 | 9        | 0.37          |
| (1,621) | 1:A:124:ILE:HD11 | 1:A:123:ARG:HA   | 1        | 0.37          |
| (1,621) | 1:A:124:ILE:HD12 | 1:A:123:ARG:HA   | 1        | 0.37          |
| (1,621) | 1:A:124:ILE:HD13 | 1:A:123:ARG:HA   | 1        | 0.37          |
| (1,609) | 1:A:123:ARG:HA   | 1:A:123:ARG:HD2  | 3        | 0.37          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,609)  | 1:A:123:ARG:HA   | 1:A:123:ARG:HD3 | 3        | 0.37          |
| (1,593)  | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA  | 1        | 0.37          |
| (1,593)  | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA  | 1        | 0.37          |
| (1,591)  | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA  | 1        | 0.37          |
| (1,591)  | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA  | 1        | 0.37          |
| (1,586)  | 1:A:121:LYS:HA   | 1:A:122:TYR:H   | 5        | 0.37          |
| (1,585)  | 1:A:121:LYS:HG2  | 1:A:121:LYS:HA  | 5        | 0.37          |
| (1,585)  | 1:A:121:LYS:HG3  | 1:A:121:LYS:HA  | 5        | 0.37          |
| (1,569)  | 1:A:119:HIS:HA   | 1:A:101:HIS:HA  | 7        | 0.37          |
| (1,539)  | 1:A:116:ARG:H    | 1:A:116:ARG:HG2 | 2        | 0.37          |
| (1,539)  | 1:A:116:ARG:H    | 1:A:116:ARG:HG3 | 2        | 0.37          |
| (1,518)  | 1:A:114:ILE:HG21 | 1:A:114:ILE:H   | 9        | 0.37          |
| (1,518)  | 1:A:114:ILE:HG22 | 1:A:114:ILE:H   | 9        | 0.37          |
| (1,518)  | 1:A:114:ILE:HG23 | 1:A:114:ILE:H   | 9        | 0.37          |
| (1,491)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3 | 1        | 0.37          |
| (1,489)  | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3 | 1        | 0.37          |
| (1,470)  | 1:A:111:HIS:HA   | 1:A:112:GLY:H   | 4        | 0.37          |
| (1,465)  | 1:A:111:HIS:HB2  | 1:A:111:HIS:H   | 9        | 0.37          |
| (1,46)   | 1:A:75:PHE:HA    | 1:A:75:PHE:HB2  | 7        | 0.37          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD2 | 2        | 0.37          |
| (1,394)  | 1:A:103:LYS:HA   | 1:A:103:LYS:HD3 | 2        | 0.37          |
| (1,330)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA  | 1        | 0.37          |
| (1,329)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA  | 1        | 0.37          |
| (1,308)  | 1:A:96:ASP:H     | 1:A:95:GLY:H    | 3        | 0.37          |
| (1,306)  | 1:A:95:GLY:HA2   | 1:A:97:VAL:H    | 6        | 0.37          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD11 | 4        | 0.37          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD12 | 4        | 0.37          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD13 | 4        | 0.37          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD21 | 4        | 0.37          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD22 | 4        | 0.37          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD23 | 4        | 0.37          |
| (1,253)  | 1:A:89:LEU:HA    | 1:A:90:LYS:H    | 3        | 0.37          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG2  | 5        | 0.37          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG3  | 5        | 0.37          |
| (1,228)  | 1:A:87:GLU:H     | 1:A:88:GLU:H    | 9        | 0.37          |
| (1,225)  | 1:A:87:GLU:H     | 1:A:88:GLU:H    | 9        | 0.37          |
| (1,191)  | 1:A:84:PHE:HD1   | 1:A:82:LYS:H    | 7        | 0.37          |
| (1,191)  | 1:A:84:PHE:HD2   | 1:A:82:LYS:H    | 7        | 0.37          |
| (1,188)  | 1:A:83:HIS:H     | 1:A:141:GLY:HA2 | 2        | 0.37          |
| (1,1671) | 1:B:144:THR:HA   | 1:B:145:VAL:H   | 3        | 0.37          |
| (1,1671) | 1:B:144:THR:HA   | 1:B:145:VAL:H   | 4        | 0.37          |
| (1,1671) | 1:B:144:THR:HA   | 1:B:145:VAL:H   | 7        | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD11 | 2        | 0.37          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD12 | 2        | 0.37          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD13 | 2        | 0.37          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD21 | 2        | 0.37          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD22 | 2        | 0.37          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD23 | 2        | 0.37          |
| (1,1611) | 1:B:135:SER:HB3  | 1:B:146:ASP:H    | 4        | 0.37          |
| (1,1540) | 1:B:127:ASP:HB3  | 1:B:128:VAL:H    | 3        | 0.37          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD11 | 2        | 0.37          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD12 | 2        | 0.37          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD13 | 2        | 0.37          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD11 | 9        | 0.37          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD12 | 9        | 0.37          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD13 | 9        | 0.37          |
| (1,1488) | 1:B:124:ILE:HD11 | 1:B:123:ARG:HA   | 1        | 0.37          |
| (1,1488) | 1:B:124:ILE:HD12 | 1:B:123:ARG:HA   | 1        | 0.37          |
| (1,1488) | 1:B:124:ILE:HD13 | 1:B:123:ARG:HA   | 1        | 0.37          |
| (1,1476) | 1:B:123:ARG:HA   | 1:B:123:ARG:HD2  | 3        | 0.37          |
| (1,1476) | 1:B:123:ARG:HA   | 1:B:123:ARG:HD3  | 3        | 0.37          |
| (1,1460) | 1:B:122:TYR:HB2  | 1:B:122:TYR:HA   | 1        | 0.37          |
| (1,1460) | 1:B:122:TYR:HB3  | 1:B:122:TYR:HA   | 1        | 0.37          |
| (1,1458) | 1:B:122:TYR:HB2  | 1:B:122:TYR:HA   | 1        | 0.37          |
| (1,1458) | 1:B:122:TYR:HB3  | 1:B:122:TYR:HA   | 1        | 0.37          |
| (1,1453) | 1:B:121:LYS:HA   | 1:B:122:TYR:H    | 5        | 0.37          |
| (1,1452) | 1:B:121:LYS:HG2  | 1:B:121:LYS:HA   | 5        | 0.37          |
| (1,1452) | 1:B:121:LYS:HG3  | 1:B:121:LYS:HA   | 5        | 0.37          |
| (1,1440) | 1:B:119:HIS:HA   | 1:B:119:HIS:HD2  | 9        | 0.37          |
| (1,1436) | 1:B:119:HIS:HA   | 1:B:101:HIS:HA   | 7        | 0.37          |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG2  | 2        | 0.37          |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG3  | 2        | 0.37          |
| (1,1385) | 1:B:114:ILE:HG21 | 1:B:114:ILE:H    | 9        | 0.37          |
| (1,1385) | 1:B:114:ILE:HG22 | 1:B:114:ILE:H    | 9        | 0.37          |
| (1,1385) | 1:B:114:ILE:HG23 | 1:B:114:ILE:H    | 9        | 0.37          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB2  | 8        | 0.37          |
| (1,1370) | 1:B:114:ILE:HD11 | 1:B:106:GLU:HB3  | 8        | 0.37          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB2  | 8        | 0.37          |
| (1,1370) | 1:B:114:ILE:HD12 | 1:B:106:GLU:HB3  | 8        | 0.37          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB2  | 8        | 0.37          |
| (1,1370) | 1:B:114:ILE:HD13 | 1:B:106:GLU:HB3  | 8        | 0.37          |
| (1,137)  | 1:A:79:LEU:HA    | 1:A:79:LEU:HG    | 5        | 0.37          |
| (1,137)  | 1:A:79:LEU:HA    | 1:A:79:LEU:HG    | 9        | 0.37          |
| (1,1358) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3  | 1        | 0.37          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1356) | 1:B:113:PHE:HA  | 1:B:113:PHE:HB3 | 1        | 0.37          |
| (1,1337) | 1:B:111:HIS:HA  | 1:B:112:GLY:H   | 4        | 0.37          |
| (1,1332) | 1:B:111:HIS:HB2 | 1:B:111:HIS:H   | 9        | 0.37          |
| (1,1304) | 1:B:107:ARG:HB2 | 1:B:113:PHE:HD1 | 5        | 0.37          |
| (1,1304) | 1:B:107:ARG:HB2 | 1:B:113:PHE:HD2 | 5        | 0.37          |
| (1,1261) | 1:B:103:LYS:HA  | 1:B:103:LYS:HD2 | 2        | 0.37          |
| (1,1261) | 1:B:103:LYS:HA  | 1:B:103:LYS:HD3 | 2        | 0.37          |
| (1,1245) | 1:B:101:HIS:HB3 | 1:B:101:HIS:H   | 6        | 0.37          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD11 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD12 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD13 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD21 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD22 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD23 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD11 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD12 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD13 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD21 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD22 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD23 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD11 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD12 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD13 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD21 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD22 | 4        | 0.37          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD23 | 4        | 0.37          |
| (1,1197) | 1:B:97:VAL:HA   | 1:B:123:ARG:HA  | 1        | 0.37          |
| (1,1196) | 1:B:97:VAL:HA   | 1:B:123:ARG:HA  | 1        | 0.37          |
| (1,118)  | 1:A:77:VAL:HB   | 1:A:146:ASP:HB2 | 1        | 0.37          |
| (1,1175) | 1:B:96:ASP:H    | 1:B:95:GLY:H    | 3        | 0.37          |
| (1,1173) | 1:B:95:GLY:HA2  | 1:B:97:VAL:H    | 6        | 0.37          |
| (1,1156) | 1:B:94:LEU:H    | 1:B:93:VAL:HB   | 8        | 0.37          |
| (1,1138) | 1:B:91:VAL:HB   | 1:B:92:LYS:H    | 4        | 0.37          |
| (1,1120) | 1:B:89:LEU:HA   | 1:B:90:LYS:H    | 3        | 0.37          |
| (1,1058) | 1:B:84:PHE:HD1  | 1:B:82:LYS:H    | 7        | 0.37          |
| (1,1058) | 1:B:84:PHE:HD2  | 1:B:82:LYS:H    | 7        | 0.37          |
| (1,1004) | 1:B:79:LEU:HA   | 1:B:79:LEU:HG   | 5        | 0.37          |
| (1,1004) | 1:B:79:LEU:HA   | 1:B:79:LEU:HG   | 9        | 0.37          |
| (1,995)  | 1:B:78:ASN:HA   | 1:B:79:LEU:H    | 6        | 0.36          |
| (1,982)  | 1:B:77:VAL:HG11 | 1:B:145:VAL:H   | 1        | 0.36          |
| (1,982)  | 1:B:77:VAL:HG12 | 1:B:145:VAL:H   | 1        | 0.36          |
| (1,982)  | 1:B:77:VAL:HG13 | 1:B:145:VAL:H   | 1        | 0.36          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,981) | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG11 | 7        | 0.36          |
| (1,981) | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG12 | 7        | 0.36          |
| (1,981) | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG13 | 7        | 0.36          |
| (1,981) | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG11 | 7        | 0.36          |
| (1,981) | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG12 | 7        | 0.36          |
| (1,981) | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG13 | 7        | 0.36          |
| (1,981) | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG11 | 7        | 0.36          |
| (1,981) | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG12 | 7        | 0.36          |
| (1,981) | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG13 | 7        | 0.36          |
| (1,955) | 1:B:77:VAL:HG11  | 1:B:76:SER:HA    | 2        | 0.36          |
| (1,955) | 1:B:77:VAL:HG12  | 1:B:76:SER:HA    | 2        | 0.36          |
| (1,955) | 1:B:77:VAL:HG13  | 1:B:76:SER:HA    | 2        | 0.36          |
| (1,892) | 1:B:71:GLU:H     | 1:B:71:GLU:HG2   | 5        | 0.36          |
| (1,892) | 1:B:71:GLU:H     | 1:B:71:GLU:HG3   | 5        | 0.36          |
| (1,88)  | 1:A:77:VAL:HG11  | 1:A:76:SER:HA    | 2        | 0.36          |
| (1,88)  | 1:A:77:VAL:HG12  | 1:A:76:SER:HA    | 2        | 0.36          |
| (1,88)  | 1:A:77:VAL:HG13  | 1:A:76:SER:HA    | 2        | 0.36          |
| (1,848) | 1:A:147:GLY:HA3  | 1:A:147:GLY:H    | 4        | 0.36          |
| (1,844) | 1:A:147:GLY:HA3  | 1:A:133:ILE:HB   | 8        | 0.36          |
| (1,827) | 1:A:146:ASP:HB3  | 1:A:76:SER:HA    | 8        | 0.36          |
| (1,826) | 1:A:146:ASP:HB3  | 1:A:76:SER:HA    | 8        | 0.36          |
| (1,819) | 1:A:145:VAL:HG21 | 1:A:145:VAL:H    | 9        | 0.36          |
| (1,819) | 1:A:145:VAL:HG22 | 1:A:145:VAL:H    | 9        | 0.36          |
| (1,819) | 1:A:145:VAL:HG23 | 1:A:145:VAL:H    | 9        | 0.36          |
| (1,804) | 1:A:144:THR:HA   | 1:A:145:VAL:H    | 5        | 0.36          |
| (1,804) | 1:A:144:THR:HA   | 1:A:145:VAL:H    | 9        | 0.36          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD11 | 1        | 0.36          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD12 | 1        | 0.36          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD13 | 1        | 0.36          |
| (1,605) | 1:A:123:ARG:HD2  | 1:A:98:ILE:H     | 9        | 0.36          |
| (1,605) | 1:A:123:ARG:HD3  | 1:A:98:ILE:H     | 9        | 0.36          |
| (1,585) | 1:A:121:LYS:HG2  | 1:A:121:LYS:HA   | 3        | 0.36          |
| (1,585) | 1:A:121:LYS:HG3  | 1:A:121:LYS:HA   | 3        | 0.36          |
| (1,544) | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 4        | 0.36          |
| (1,543) | 1:A:117:GLU:HA   | 1:A:103:LYS:HA   | 4        | 0.36          |
| (1,491) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 2        | 0.36          |
| (1,491) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 9        | 0.36          |
| (1,489) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 2        | 0.36          |
| (1,489) | 1:A:113:PHE:HA   | 1:A:113:PHE:HB3  | 9        | 0.36          |
| (1,470) | 1:A:111:HIS:HA   | 1:A:112:GLY:H    | 8        | 0.36          |
| (1,392) | 1:A:102:GLY:H    | 1:A:118:PHE:H    | 2        | 0.36          |
| (1,354) | 1:A:99:GLU:HA    | 1:A:100:VAL:H    | 4        | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,351)  | 1:A:99:GLU:HA    | 1:A:99:GLU:H     | 9        | 0.36          |
| (1,330)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA   | 2        | 0.36          |
| (1,329)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA   | 2        | 0.36          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD11  | 7        | 0.36          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD12  | 7        | 0.36          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD13  | 7        | 0.36          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD21  | 7        | 0.36          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD22  | 7        | 0.36          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD23  | 7        | 0.36          |
| (1,285)  | 1:A:93:VAL:HG11  | 1:A:93:VAL:H     | 7        | 0.36          |
| (1,285)  | 1:A:93:VAL:HG12  | 1:A:93:VAL:H     | 7        | 0.36          |
| (1,285)  | 1:A:93:VAL:HG13  | 1:A:93:VAL:H     | 7        | 0.36          |
| (1,285)  | 1:A:93:VAL:HG21  | 1:A:93:VAL:H     | 7        | 0.36          |
| (1,285)  | 1:A:93:VAL:HG22  | 1:A:93:VAL:H     | 7        | 0.36          |
| (1,285)  | 1:A:93:VAL:HG23  | 1:A:93:VAL:H     | 7        | 0.36          |
| (1,271)  | 1:A:91:VAL:HB    | 1:A:92:LYS:H     | 4        | 0.36          |
| (1,251)  | 1:A:89:LEU:HG    | 1:A:90:LYS:H     | 5        | 0.36          |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD21  | 9        | 0.36          |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD22  | 9        | 0.36          |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD23  | 9        | 0.36          |
| (1,238)  | 1:A:89:LEU:HD11  | 1:A:85:SER:H     | 3        | 0.36          |
| (1,238)  | 1:A:89:LEU:HD12  | 1:A:85:SER:H     | 3        | 0.36          |
| (1,238)  | 1:A:89:LEU:HD13  | 1:A:85:SER:H     | 3        | 0.36          |
| (1,231)  | 1:A:87:GLU:HB2   | 1:A:89:LEU:H     | 3        | 0.36          |
| (1,231)  | 1:A:87:GLU:HB3   | 1:A:89:LEU:H     | 3        | 0.36          |
| (1,212)  | 1:A:85:SER:HB2   | 1:A:88:GLU:H     | 7        | 0.36          |
| (1,212)  | 1:A:85:SER:HB2   | 1:A:88:GLU:H     | 8        | 0.36          |
| (1,200)  | 1:A:84:PHE:HD1   | 1:A:85:SER:H     | 5        | 0.36          |
| (1,200)  | 1:A:84:PHE:HD2   | 1:A:85:SER:H     | 5        | 0.36          |
| (1,1715) | 1:B:147:GLY:HA3  | 1:B:147:GLY:H    | 4        | 0.36          |
| (1,1711) | 1:B:147:GLY:HA3  | 1:B:133:ILE:HB   | 8        | 0.36          |
| (1,1694) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA    | 8        | 0.36          |
| (1,1693) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA    | 8        | 0.36          |
| (1,1686) | 1:B:145:VAL:HG21 | 1:B:145:VAL:H    | 9        | 0.36          |
| (1,1686) | 1:B:145:VAL:HG22 | 1:B:145:VAL:H    | 9        | 0.36          |
| (1,1686) | 1:B:145:VAL:HG23 | 1:B:145:VAL:H    | 9        | 0.36          |
| (1,1671) | 1:B:144:THR:HA   | 1:B:145:VAL:H    | 5        | 0.36          |
| (1,1671) | 1:B:144:THR:HA   | 1:B:145:VAL:H    | 8        | 0.36          |
| (1,1671) | 1:B:144:THR:HA   | 1:B:145:VAL:H    | 9        | 0.36          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG11 | 7        | 0.36          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG12 | 7        | 0.36          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG13 | 7        | 0.36          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1646) | 1:B:142:VAL:HA  | 1:B:142:VAL:HG21 | 7        | 0.36          |
| (1,1646) | 1:B:142:VAL:HA  | 1:B:142:VAL:HG22 | 7        | 0.36          |
| (1,1646) | 1:B:142:VAL:HA  | 1:B:142:VAL:HG23 | 7        | 0.36          |
| (1,1514) | 1:B:125:PRO:HD3 | 1:B:124:ILE:HD11 | 1        | 0.36          |
| (1,1514) | 1:B:125:PRO:HD3 | 1:B:124:ILE:HD12 | 1        | 0.36          |
| (1,1514) | 1:B:125:PRO:HD3 | 1:B:124:ILE:HD13 | 1        | 0.36          |
| (1,1514) | 1:B:125:PRO:HD3 | 1:B:124:ILE:HD11 | 6        | 0.36          |
| (1,1514) | 1:B:125:PRO:HD3 | 1:B:124:ILE:HD12 | 6        | 0.36          |
| (1,1514) | 1:B:125:PRO:HD3 | 1:B:124:ILE:HD13 | 6        | 0.36          |
| (1,1472) | 1:B:123:ARG:HD2 | 1:B:98:ILE:H     | 9        | 0.36          |
| (1,1472) | 1:B:123:ARG:HD3 | 1:B:98:ILE:H     | 9        | 0.36          |
| (1,1452) | 1:B:121:LYS:HG2 | 1:B:121:LYS:HA   | 3        | 0.36          |
| (1,1452) | 1:B:121:LYS:HG3 | 1:B:121:LYS:HA   | 3        | 0.36          |
| (1,1411) | 1:B:117:GLU:HA  | 1:B:103:LYS:HA   | 4        | 0.36          |
| (1,1410) | 1:B:117:GLU:HA  | 1:B:103:LYS:HA   | 4        | 0.36          |
| (1,14)   | 1:A:68:MET:HE1  | 1:A:122:TYR:HD1  | 2        | 0.36          |
| (1,14)   | 1:A:68:MET:HE1  | 1:A:122:TYR:HD2  | 2        | 0.36          |
| (1,14)   | 1:A:68:MET:HE2  | 1:A:122:TYR:HD1  | 2        | 0.36          |
| (1,14)   | 1:A:68:MET:HE2  | 1:A:122:TYR:HD2  | 2        | 0.36          |
| (1,14)   | 1:A:68:MET:HE3  | 1:A:122:TYR:HD1  | 2        | 0.36          |
| (1,14)   | 1:A:68:MET:HE3  | 1:A:122:TYR:HD2  | 2        | 0.36          |
| (1,1358) | 1:B:113:PHE:HA  | 1:B:113:PHE:HB3  | 9        | 0.36          |
| (1,1356) | 1:B:113:PHE:HA  | 1:B:113:PHE:HB3  | 9        | 0.36          |
| (1,1337) | 1:B:111:HIS:HA  | 1:B:112:GLY:H    | 8        | 0.36          |
| (1,128)  | 1:A:78:ASN:HA   | 1:A:79:LEU:H     | 6        | 0.36          |
| (1,1259) | 1:B:102:GLY:H   | 1:B:118:PHE:H    | 2        | 0.36          |
| (1,1218) | 1:B:99:GLU:HA   | 1:B:99:GLU:H     | 9        | 0.36          |
| (1,1197) | 1:B:97:VAL:HA   | 1:B:123:ARG:HA   | 2        | 0.36          |
| (1,1196) | 1:B:97:VAL:HA   | 1:B:123:ARG:HA   | 2        | 0.36          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD11  | 7        | 0.36          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD12  | 7        | 0.36          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD13  | 7        | 0.36          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD21  | 7        | 0.36          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD22  | 7        | 0.36          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD23  | 7        | 0.36          |
| (1,1152) | 1:B:93:VAL:HG11 | 1:B:93:VAL:H     | 7        | 0.36          |
| (1,1152) | 1:B:93:VAL:HG12 | 1:B:93:VAL:H     | 7        | 0.36          |
| (1,1152) | 1:B:93:VAL:HG13 | 1:B:93:VAL:H     | 7        | 0.36          |
| (1,1152) | 1:B:93:VAL:HG21 | 1:B:93:VAL:H     | 7        | 0.36          |
| (1,1152) | 1:B:93:VAL:HG22 | 1:B:93:VAL:H     | 7        | 0.36          |
| (1,1152) | 1:B:93:VAL:HG23 | 1:B:93:VAL:H     | 7        | 0.36          |
| (1,1152) | 1:B:93:VAL:HG11 | 1:B:93:VAL:H     | 9        | 0.36          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1152) | 1:B:93:VAL:HG12 | 1:B:93:VAL:H     | 9        | 0.36          |
| (1,1152) | 1:B:93:VAL:HG13 | 1:B:93:VAL:H     | 9        | 0.36          |
| (1,1152) | 1:B:93:VAL:HG21 | 1:B:93:VAL:H     | 9        | 0.36          |
| (1,1152) | 1:B:93:VAL:HG22 | 1:B:93:VAL:H     | 9        | 0.36          |
| (1,1152) | 1:B:93:VAL:HG23 | 1:B:93:VAL:H     | 9        | 0.36          |
| (1,115)  | 1:A:77:VAL:HG11 | 1:A:145:VAL:H    | 1        | 0.36          |
| (1,115)  | 1:A:77:VAL:HG12 | 1:A:145:VAL:H    | 1        | 0.36          |
| (1,115)  | 1:A:77:VAL:HG13 | 1:A:145:VAL:H    | 1        | 0.36          |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG11 | 7        | 0.36          |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG12 | 7        | 0.36          |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG13 | 7        | 0.36          |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG11 | 7        | 0.36          |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG12 | 7        | 0.36          |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG13 | 7        | 0.36          |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG11 | 7        | 0.36          |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG12 | 7        | 0.36          |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG13 | 7        | 0.36          |
| (1,1118) | 1:B:89:LEU:HG   | 1:B:90:LYS:H     | 5        | 0.36          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD21  | 9        | 0.36          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD22  | 9        | 0.36          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD23  | 9        | 0.36          |
| (1,1105) | 1:B:89:LEU:HD11 | 1:B:85:SER:H     | 3        | 0.36          |
| (1,1105) | 1:B:89:LEU:HD12 | 1:B:85:SER:H     | 3        | 0.36          |
| (1,1105) | 1:B:89:LEU:HD13 | 1:B:85:SER:H     | 3        | 0.36          |
| (1,1098) | 1:B:87:GLU:HB2  | 1:B:89:LEU:H     | 3        | 0.36          |
| (1,1098) | 1:B:87:GLU:HB3  | 1:B:89:LEU:H     | 3        | 0.36          |
| (1,1095) | 1:B:87:GLU:H    | 1:B:88:GLU:H     | 9        | 0.36          |
| (1,1092) | 1:B:87:GLU:H    | 1:B:88:GLU:H     | 9        | 0.36          |
| (1,1079) | 1:B:85:SER:HB2  | 1:B:88:GLU:H     | 7        | 0.36          |
| (1,1079) | 1:B:85:SER:HB2  | 1:B:88:GLU:H     | 8        | 0.36          |
| (1,1067) | 1:B:84:PHE:HD1  | 1:B:85:SER:H     | 5        | 0.36          |
| (1,1067) | 1:B:84:PHE:HD2  | 1:B:85:SER:H     | 5        | 0.36          |
| (1,1055) | 1:B:83:HIS:H    | 1:B:141:GLY:HA2  | 2        | 0.36          |
| (1,995)  | 1:B:78:ASN:HA   | 1:B:79:LEU:H     | 3        | 0.35          |
| (1,995)  | 1:B:78:ASN:HA   | 1:B:79:LEU:H     | 5        | 0.35          |
| (1,995)  | 1:B:78:ASN:HA   | 1:B:79:LEU:H     | 9        | 0.35          |
| (1,967)  | 1:B:77:VAL:HG11 | 1:B:78:ASN:HB2   | 6        | 0.35          |
| (1,967)  | 1:B:77:VAL:HG12 | 1:B:78:ASN:HB2   | 6        | 0.35          |
| (1,967)  | 1:B:77:VAL:HG13 | 1:B:78:ASN:HB2   | 6        | 0.35          |
| (1,945)  | 1:B:76:SER:HA   | 1:B:146:ASP:HA   | 1        | 0.35          |
| (1,941)  | 1:B:76:SER:HA   | 1:B:146:ASP:HA   | 1        | 0.35          |
| (1,892)  | 1:B:71:GLU:H    | 1:B:71:GLU:HG2   | 4        | 0.35          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,892) | 1:B:71:GLU:H     | 1:B:71:GLU:HG3   | 4        | 0.35          |
| (1,857) | 1:A:150:LYS:H    | 1:A:150:LYS:HD2  | 5        | 0.35          |
| (1,857) | 1:A:150:LYS:H    | 1:A:150:LYS:HD3  | 5        | 0.35          |
| (1,857) | 1:A:150:LYS:H    | 1:A:150:LYS:HD2  | 9        | 0.35          |
| (1,857) | 1:A:150:LYS:H    | 1:A:150:LYS:HD3  | 9        | 0.35          |
| (1,812) | 1:A:145:VAL:HB   | 1:A:135:SER:HA   | 7        | 0.35          |
| (1,804) | 1:A:144:THR:HA   | 1:A:145:VAL:H    | 8        | 0.35          |
| (1,787) | 1:A:143:LEU:H    | 1:A:79:LEU:H     | 1        | 0.35          |
| (1,78)  | 1:A:76:SER:HA    | 1:A:146:ASP:HA   | 1        | 0.35          |
| (1,74)  | 1:A:76:SER:HA    | 1:A:146:ASP:HA   | 1        | 0.35          |
| (1,719) | 1:A:133:ILE:HG21 | 1:A:133:ILE:HA   | 5        | 0.35          |
| (1,719) | 1:A:133:ILE:HG22 | 1:A:133:ILE:HA   | 5        | 0.35          |
| (1,719) | 1:A:133:ILE:HG23 | 1:A:133:ILE:HA   | 5        | 0.35          |
| (1,719) | 1:A:133:ILE:HG21 | 1:A:133:ILE:HA   | 9        | 0.35          |
| (1,719) | 1:A:133:ILE:HG22 | 1:A:133:ILE:HA   | 9        | 0.35          |
| (1,719) | 1:A:133:ILE:HG23 | 1:A:133:ILE:HA   | 9        | 0.35          |
| (1,673) | 1:A:127:ASP:HB3  | 1:A:128:VAL:H    | 5        | 0.35          |
| (1,673) | 1:A:127:ASP:HB3  | 1:A:128:VAL:H    | 7        | 0.35          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD11 | 6        | 0.35          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD12 | 6        | 0.35          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD13 | 6        | 0.35          |
| (1,578) | 1:A:119:HIS:HA   | 1:A:119:HIS:H    | 6        | 0.35          |
| (1,578) | 1:A:119:HIS:HA   | 1:A:119:HIS:H    | 7        | 0.35          |
| (1,578) | 1:A:119:HIS:HA   | 1:A:119:HIS:H    | 9        | 0.35          |
| (1,563) | 1:A:118:PHE:HB2  | 1:A:118:PHE:H    | 7        | 0.35          |
| (1,550) | 1:A:118:PHE:HE1  | 1:A:102:GLY:H    | 9        | 0.35          |
| (1,550) | 1:A:118:PHE:HE2  | 1:A:102:GLY:H    | 9        | 0.35          |
| (1,512) | 1:A:114:ILE:HD11 | 1:A:113:PHE:HA   | 9        | 0.35          |
| (1,512) | 1:A:114:ILE:HD12 | 1:A:113:PHE:HA   | 9        | 0.35          |
| (1,512) | 1:A:114:ILE:HD13 | 1:A:113:PHE:HA   | 9        | 0.35          |
| (1,457) | 1:A:111:HIS:H    | 1:A:109:ASP:HB2  | 9        | 0.35          |
| (1,457) | 1:A:111:HIS:H    | 1:A:109:ASP:HB3  | 9        | 0.35          |
| (1,430) | 1:A:107:ARG:H    | 1:A:108:GLN:H    | 3        | 0.35          |
| (1,426) | 1:A:107:ARG:HD2  | 1:A:107:ARG:H    | 8        | 0.35          |
| (1,387) | 1:A:102:GLY:HA3  | 1:A:102:GLY:H    | 2        | 0.35          |
| (1,378) | 1:A:101:HIS:HB3  | 1:A:101:HIS:H    | 3        | 0.35          |
| (1,289) | 1:A:94:LEU:H     | 1:A:93:VAL:HB    | 7        | 0.35          |
| (1,287) | 1:A:93:VAL:HA    | 1:A:98:ILE:HA    | 7        | 0.35          |
| (1,285) | 1:A:93:VAL:HG11  | 1:A:93:VAL:H     | 4        | 0.35          |
| (1,285) | 1:A:93:VAL:HG12  | 1:A:93:VAL:H     | 4        | 0.35          |
| (1,285) | 1:A:93:VAL:HG13  | 1:A:93:VAL:H     | 4        | 0.35          |
| (1,285) | 1:A:93:VAL:HG21  | 1:A:93:VAL:H     | 4        | 0.35          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,285)  | 1:A:93:VAL:HG22  | 1:A:93:VAL:H    | 4        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG23  | 1:A:93:VAL:H    | 4        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG11  | 1:A:93:VAL:H    | 6        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG12  | 1:A:93:VAL:H    | 6        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG13  | 1:A:93:VAL:H    | 6        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG21  | 1:A:93:VAL:H    | 6        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG22  | 1:A:93:VAL:H    | 6        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG23  | 1:A:93:VAL:H    | 6        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG11  | 1:A:93:VAL:H    | 9        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG12  | 1:A:93:VAL:H    | 9        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG13  | 1:A:93:VAL:H    | 9        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG21  | 1:A:93:VAL:H    | 9        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG22  | 1:A:93:VAL:H    | 9        | 0.35          |
| (1,285)  | 1:A:93:VAL:HG23  | 1:A:93:VAL:H    | 9        | 0.35          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG2  | 4        | 0.35          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG3  | 4        | 0.35          |
| (1,226)  | 1:A:87:GLU:HG2   | 1:A:88:GLU:H    | 4        | 0.35          |
| (1,226)  | 1:A:87:GLU:HG3   | 1:A:88:GLU:H    | 4        | 0.35          |
| (1,226)  | 1:A:87:GLU:HG2   | 1:A:88:GLU:H    | 7        | 0.35          |
| (1,226)  | 1:A:87:GLU:HG3   | 1:A:88:GLU:H    | 7        | 0.35          |
| (1,212)  | 1:A:85:SER:HB2   | 1:A:88:GLU:H    | 3        | 0.35          |
| (1,1768) | 1:A:122:TYR:HA   | 1:B:112:GLY:H   | 3        | 0.35          |
| (1,1753) | 1:A:118:PHE:HA   | 1:B:116:ARG:HA  | 1        | 0.35          |
| (1,1738) | 1:A:111:HIS:HA   | 1:B:122:TYR:HD1 | 1        | 0.35          |
| (1,1738) | 1:A:111:HIS:HA   | 1:B:122:TYR:HD2 | 1        | 0.35          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD2 | 5        | 0.35          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD3 | 5        | 0.35          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD2 | 9        | 0.35          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD3 | 9        | 0.35          |
| (1,1679) | 1:B:145:VAL:HB   | 1:B:135:SER:HA  | 7        | 0.35          |
| (1,1654) | 1:B:143:LEU:H    | 1:B:79:LEU:H    | 1        | 0.35          |
| (1,1586) | 1:B:133:ILE:HG21 | 1:B:133:ILE:HA  | 5        | 0.35          |
| (1,1586) | 1:B:133:ILE:HG22 | 1:B:133:ILE:HA  | 5        | 0.35          |
| (1,1586) | 1:B:133:ILE:HG23 | 1:B:133:ILE:HA  | 5        | 0.35          |
| (1,1586) | 1:B:133:ILE:HG21 | 1:B:133:ILE:HA  | 9        | 0.35          |
| (1,1586) | 1:B:133:ILE:HG22 | 1:B:133:ILE:HA  | 9        | 0.35          |
| (1,1586) | 1:B:133:ILE:HG23 | 1:B:133:ILE:HA  | 9        | 0.35          |
| (1,1540) | 1:B:127:ASP:HB3  | 1:B:128:VAL:H   | 5        | 0.35          |
| (1,1540) | 1:B:127:ASP:HB3  | 1:B:128:VAL:H   | 7        | 0.35          |
| (1,1445) | 1:B:119:HIS:HA   | 1:B:119:HIS:H   | 6        | 0.35          |
| (1,1445) | 1:B:119:HIS:HA   | 1:B:119:HIS:H   | 7        | 0.35          |
| (1,1445) | 1:B:119:HIS:HA   | 1:B:119:HIS:H   | 9        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1430) | 1:B:118:PHE:HB2  | 1:B:118:PHE:H    | 7        | 0.35          |
| (1,1417) | 1:B:118:PHE:HE1  | 1:B:102:GLY:H    | 9        | 0.35          |
| (1,1417) | 1:B:118:PHE:HE2  | 1:B:102:GLY:H    | 9        | 0.35          |
| (1,1379) | 1:B:114:ILE:HD11 | 1:B:113:PHE:HA   | 9        | 0.35          |
| (1,1379) | 1:B:114:ILE:HD12 | 1:B:113:PHE:HA   | 9        | 0.35          |
| (1,1379) | 1:B:114:ILE:HD13 | 1:B:113:PHE:HA   | 9        | 0.35          |
| (1,1358) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3  | 2        | 0.35          |
| (1,1356) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3  | 2        | 0.35          |
| (1,1324) | 1:B:111:HIS:H    | 1:B:109:ASP:HB2  | 9        | 0.35          |
| (1,1324) | 1:B:111:HIS:H    | 1:B:109:ASP:HB3  | 9        | 0.35          |
| (1,1297) | 1:B:107:ARG:H    | 1:B:108:GLN:H    | 3        | 0.35          |
| (1,1293) | 1:B:107:ARG:HD2  | 1:B:107:ARG:H    | 8        | 0.35          |
| (1,128)  | 1:A:78:ASN:HA    | 1:A:79:LEU:H     | 3        | 0.35          |
| (1,128)  | 1:A:78:ASN:HA    | 1:A:79:LEU:H     | 5        | 0.35          |
| (1,1254) | 1:B:102:GLY:HA3  | 1:B:102:GLY:H    | 2        | 0.35          |
| (1,1245) | 1:B:101:HIS:HB3  | 1:B:101:HIS:H    | 3        | 0.35          |
| (1,1221) | 1:B:99:GLU:HA    | 1:B:100:VAL:H    | 4        | 0.35          |
| (1,1156) | 1:B:94:LEU:H     | 1:B:93:VAL:HB    | 7        | 0.35          |
| (1,1154) | 1:B:93:VAL:HA    | 1:B:98:ILE:HA    | 7        | 0.35          |
| (1,1152) | 1:B:93:VAL:HG11  | 1:B:93:VAL:H     | 6        | 0.35          |
| (1,1152) | 1:B:93:VAL:HG12  | 1:B:93:VAL:H     | 6        | 0.35          |
| (1,1152) | 1:B:93:VAL:HG13  | 1:B:93:VAL:H     | 6        | 0.35          |
| (1,1152) | 1:B:93:VAL:HG21  | 1:B:93:VAL:H     | 6        | 0.35          |
| (1,1152) | 1:B:93:VAL:HG22  | 1:B:93:VAL:H     | 6        | 0.35          |
| (1,1152) | 1:B:93:VAL:HG23  | 1:B:93:VAL:H     | 6        | 0.35          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG11 | 4        | 0.35          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG12 | 4        | 0.35          |
| (1,114)  | 1:A:77:VAL:HG21  | 1:A:145:VAL:HG13 | 4        | 0.35          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG11 | 4        | 0.35          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG12 | 4        | 0.35          |
| (1,114)  | 1:A:77:VAL:HG22  | 1:A:145:VAL:HG13 | 4        | 0.35          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG11 | 4        | 0.35          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG12 | 4        | 0.35          |
| (1,114)  | 1:A:77:VAL:HG23  | 1:A:145:VAL:HG13 | 4        | 0.35          |
| (1,1093) | 1:B:87:GLU:HG2   | 1:B:88:GLU:H     | 4        | 0.35          |
| (1,1093) | 1:B:87:GLU:HG3   | 1:B:88:GLU:H     | 4        | 0.35          |
| (1,1093) | 1:B:87:GLU:HG2   | 1:B:88:GLU:H     | 7        | 0.35          |
| (1,1093) | 1:B:87:GLU:HG3   | 1:B:88:GLU:H     | 7        | 0.35          |
| (1,1079) | 1:B:85:SER:HB2   | 1:B:88:GLU:H     | 3        | 0.35          |
| (1,1065) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H     | 4        | 0.35          |
| (1,1065) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H     | 4        | 0.35          |
| (1,1063) | 1:B:84:PHE:HB2   | 1:B:84:PHE:H     | 4        | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1063) | 1:B:84:PHE:HB3   | 1:B:84:PHE:H     | 4        | 0.35          |
| (1,100)  | 1:A:77:VAL:HG11  | 1:A:78:ASN:HB2   | 6        | 0.35          |
| (1,100)  | 1:A:77:VAL:HG12  | 1:A:78:ASN:HB2   | 6        | 0.35          |
| (1,100)  | 1:A:77:VAL:HG13  | 1:A:78:ASN:HB2   | 6        | 0.35          |
| (1,995)  | 1:B:78:ASN:HA    | 1:B:79:LEU:H     | 7        | 0.34          |
| (1,981)  | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG11 | 4        | 0.34          |
| (1,981)  | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG12 | 4        | 0.34          |
| (1,981)  | 1:B:77:VAL:HG21  | 1:B:145:VAL:HG13 | 4        | 0.34          |
| (1,981)  | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG11 | 4        | 0.34          |
| (1,981)  | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG12 | 4        | 0.34          |
| (1,981)  | 1:B:77:VAL:HG22  | 1:B:145:VAL:HG13 | 4        | 0.34          |
| (1,981)  | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG11 | 4        | 0.34          |
| (1,981)  | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG12 | 4        | 0.34          |
| (1,981)  | 1:B:77:VAL:HG23  | 1:B:145:VAL:HG13 | 4        | 0.34          |
| (1,975)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:H     | 8        | 0.34          |
| (1,975)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:H     | 8        | 0.34          |
| (1,975)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:H     | 8        | 0.34          |
| (1,929)  | 1:B:76:SER:HB3   | 1:B:76:SER:H     | 9        | 0.34          |
| (1,909)  | 1:B:74:ARG:H     | 1:B:74:ARG:HB2   | 9        | 0.34          |
| (1,872)  | 1:B:67:GLU:H     | 1:B:67:GLU:HA    | 4        | 0.34          |
| (1,825)  | 1:A:146:ASP:HB2  | 1:A:76:SER:HA    | 1        | 0.34          |
| (1,825)  | 1:A:146:ASP:HB2  | 1:A:76:SER:HA    | 9        | 0.34          |
| (1,824)  | 1:A:146:ASP:HB2  | 1:A:76:SER:HA    | 1        | 0.34          |
| (1,824)  | 1:A:146:ASP:HB2  | 1:A:76:SER:HA    | 9        | 0.34          |
| (1,804)  | 1:A:144:THR:HA   | 1:A:145:VAL:H    | 1        | 0.34          |
| (1,804)  | 1:A:144:THR:HA   | 1:A:145:VAL:H    | 6        | 0.34          |
| (1,783)  | 1:A:142:VAL:HG11 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,783)  | 1:A:142:VAL:HG12 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,783)  | 1:A:142:VAL:HG13 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,783)  | 1:A:142:VAL:HG21 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,783)  | 1:A:142:VAL:HG22 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,783)  | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,782)  | 1:A:142:VAL:HG11 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,782)  | 1:A:142:VAL:HG12 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,782)  | 1:A:142:VAL:HG13 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,782)  | 1:A:142:VAL:HG21 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,782)  | 1:A:142:VAL:HG22 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,782)  | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 4        | 0.34          |
| (1,719)  | 1:A:133:ILE:HG21 | 1:A:133:ILE:HA   | 6        | 0.34          |
| (1,719)  | 1:A:133:ILE:HG22 | 1:A:133:ILE:HA   | 6        | 0.34          |
| (1,719)  | 1:A:133:ILE:HG23 | 1:A:133:ILE:HA   | 6        | 0.34          |
| (1,62)   | 1:A:76:SER:HB3   | 1:A:76:SER:H     | 9        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,590)  | 1:A:122:TYR:HA   | 1:A:98:ILE:H     | 5        | 0.34          |
| (1,585)  | 1:A:121:LYS:HG2  | 1:A:121:LYS:HA   | 7        | 0.34          |
| (1,585)  | 1:A:121:LYS:HG3  | 1:A:121:LYS:HA   | 7        | 0.34          |
| (1,578)  | 1:A:119:HIS:HA   | 1:A:119:HIS:H    | 4        | 0.34          |
| (1,518)  | 1:A:114:ILE:HG21 | 1:A:114:ILE:H    | 7        | 0.34          |
| (1,518)  | 1:A:114:ILE:HG22 | 1:A:114:ILE:H    | 7        | 0.34          |
| (1,518)  | 1:A:114:ILE:HG23 | 1:A:114:ILE:H    | 7        | 0.34          |
| (1,42)   | 1:A:74:ARG:H     | 1:A:74:ARG:HB2   | 9        | 0.34          |
| (1,369)  | 1:A:101:HIS:H    | 1:A:100:VAL:HA   | 2        | 0.34          |
| (1,367)  | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB2   | 9        | 0.34          |
| (1,367)  | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB3   | 9        | 0.34          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG21  | 8        | 0.34          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG22  | 8        | 0.34          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG23  | 8        | 0.34          |
| (1,253)  | 1:A:89:LEU:HA    | 1:A:90:LYS:H     | 2        | 0.34          |
| (1,226)  | 1:A:87:GLU:HG2   | 1:A:88:GLU:H     | 8        | 0.34          |
| (1,226)  | 1:A:87:GLU:HG3   | 1:A:88:GLU:H     | 8        | 0.34          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD21  | 9        | 0.34          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD22  | 9        | 0.34          |
| (1,219)  | 1:A:86:PRO:HB2   | 1:A:89:LEU:HD23  | 9        | 0.34          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD21  | 9        | 0.34          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD22  | 9        | 0.34          |
| (1,219)  | 1:A:86:PRO:HB3   | 1:A:89:LEU:HD23  | 9        | 0.34          |
| (1,199)  | 1:A:84:PHE:HB2   | 1:A:85:SER:H     | 4        | 0.34          |
| (1,199)  | 1:A:84:PHE:HB3   | 1:A:85:SER:H     | 4        | 0.34          |
| (1,198)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 4        | 0.34          |
| (1,198)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 4        | 0.34          |
| (1,196)  | 1:A:84:PHE:HB2   | 1:A:84:PHE:H     | 4        | 0.34          |
| (1,196)  | 1:A:84:PHE:HB3   | 1:A:84:PHE:H     | 4        | 0.34          |
| (1,1763) | 1:A:122:TYR:HA   | 1:B:112:GLY:HA3  | 5        | 0.34          |
| (1,1756) | 1:A:118:PHE:HA   | 1:B:117:GLU:H    | 2        | 0.34          |
| (1,1736) | 1:A:111:HIS:HB2  | 1:B:122:TYR:HE1  | 4        | 0.34          |
| (1,1736) | 1:A:111:HIS:HB2  | 1:B:122:TYR:HE2  | 4        | 0.34          |
| (1,173)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HD2   | 5        | 0.34          |
| (1,1692) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA    | 1        | 0.34          |
| (1,1692) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA    | 9        | 0.34          |
| (1,1691) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA    | 1        | 0.34          |
| (1,1691) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA    | 9        | 0.34          |
| (1,1671) | 1:B:144:THR:HA   | 1:B:145:VAL:H    | 1        | 0.34          |
| (1,1671) | 1:B:144:THR:HA   | 1:B:145:VAL:H    | 6        | 0.34          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG11 | 4        | 0.34          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG12 | 4        | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG13 | 4        | 0.34          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG21 | 4        | 0.34          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG22 | 4        | 0.34          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG23 | 4        | 0.34          |
| (1,1586) | 1:B:133:ILE:HG21 | 1:B:133:ILE:HA   | 6        | 0.34          |
| (1,1586) | 1:B:133:ILE:HG22 | 1:B:133:ILE:HA   | 6        | 0.34          |
| (1,1586) | 1:B:133:ILE:HG23 | 1:B:133:ILE:HA   | 6        | 0.34          |
| (1,1476) | 1:B:123:ARG:HA   | 1:B:123:ARG:HD2  | 6        | 0.34          |
| (1,1476) | 1:B:123:ARG:HA   | 1:B:123:ARG:HD3  | 6        | 0.34          |
| (1,1457) | 1:B:122:TYR:HA   | 1:B:98:ILE:H     | 5        | 0.34          |
| (1,1452) | 1:B:121:LYS:HG2  | 1:B:121:LYS:HA   | 7        | 0.34          |
| (1,1452) | 1:B:121:LYS:HG3  | 1:B:121:LYS:HA   | 7        | 0.34          |
| (1,1445) | 1:B:119:HIS:HA   | 1:B:119:HIS:H    | 4        | 0.34          |
| (1,1385) | 1:B:114:ILE:HG21 | 1:B:114:ILE:H    | 7        | 0.34          |
| (1,1385) | 1:B:114:ILE:HG22 | 1:B:114:ILE:H    | 7        | 0.34          |
| (1,1385) | 1:B:114:ILE:HG23 | 1:B:114:ILE:H    | 7        | 0.34          |
| (1,128)  | 1:A:78:ASN:HA    | 1:A:79:LEU:H     | 7        | 0.34          |
| (1,128)  | 1:A:78:ASN:HA    | 1:A:79:LEU:H     | 9        | 0.34          |
| (1,1236) | 1:B:101:HIS:H    | 1:B:100:VAL:HA   | 2        | 0.34          |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB2   | 9        | 0.34          |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB3   | 9        | 0.34          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG21  | 8        | 0.34          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG22  | 8        | 0.34          |
| (1,1135) | 1:B:91:VAL:H     | 1:B:91:VAL:HG23  | 8        | 0.34          |
| (1,1120) | 1:B:89:LEU:HA    | 1:B:90:LYS:H     | 2        | 0.34          |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD21  | 9        | 0.34          |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD22  | 9        | 0.34          |
| (1,1086) | 1:B:86:PRO:HB2   | 1:B:89:LEU:HD23  | 9        | 0.34          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD21  | 9        | 0.34          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD22  | 9        | 0.34          |
| (1,1086) | 1:B:86:PRO:HB3   | 1:B:89:LEU:HD23  | 9        | 0.34          |
| (1,108)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:H     | 8        | 0.34          |
| (1,108)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:H     | 8        | 0.34          |
| (1,108)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:H     | 8        | 0.34          |
| (1,1066) | 1:B:84:PHE:HB2   | 1:B:85:SER:H     | 4        | 0.34          |
| (1,1066) | 1:B:84:PHE:HB3   | 1:B:85:SER:H     | 4        | 0.34          |
| (1,995)  | 1:B:78:ASN:HA    | 1:B:79:LEU:H     | 2        | 0.33          |
| (1,950)  | 1:B:77:VAL:HG11  | 1:B:68:MET:HA    | 4        | 0.33          |
| (1,950)  | 1:B:77:VAL:HG12  | 1:B:68:MET:HA    | 4        | 0.33          |
| (1,950)  | 1:B:77:VAL:HG13  | 1:B:68:MET:HA    | 4        | 0.33          |
| (1,880)  | 1:B:68:MET:HE1   | 1:B:122:TYR:HE1  | 6        | 0.33          |
| (1,880)  | 1:B:68:MET:HE1   | 1:B:122:TYR:HE2  | 6        | 0.33          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,880) | 1:B:68:MET:HE2   | 1:B:122:TYR:HE1  | 6        | 0.33          |
| (1,880) | 1:B:68:MET:HE2   | 1:B:122:TYR:HE2  | 6        | 0.33          |
| (1,880) | 1:B:68:MET:HE3   | 1:B:122:TYR:HE1  | 6        | 0.33          |
| (1,880) | 1:B:68:MET:HE3   | 1:B:122:TYR:HE2  | 6        | 0.33          |
| (1,872) | 1:B:67:GLU:H     | 1:B:67:GLU:HA    | 5        | 0.33          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD11  | 4        | 0.33          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD12  | 4        | 0.33          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD13  | 4        | 0.33          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD21  | 4        | 0.33          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD22  | 4        | 0.33          |
| (1,871) | 1:B:66:SER:HA    | 1:B:79:LEU:HD23  | 4        | 0.33          |
| (1,857) | 1:A:150:LYS:H    | 1:A:150:LYS:HD2  | 4        | 0.33          |
| (1,857) | 1:A:150:LYS:H    | 1:A:150:LYS:HD3  | 4        | 0.33          |
| (1,838) | 1:A:146:ASP:HB3  | 1:A:146:ASP:H    | 6        | 0.33          |
| (1,83)  | 1:A:77:VAL:HG11  | 1:A:68:MET:HA    | 4        | 0.33          |
| (1,83)  | 1:A:77:VAL:HG12  | 1:A:68:MET:HA    | 4        | 0.33          |
| (1,83)  | 1:A:77:VAL:HG13  | 1:A:68:MET:HA    | 4        | 0.33          |
| (1,827) | 1:A:146:ASP:HB3  | 1:A:76:SER:HA    | 3        | 0.33          |
| (1,826) | 1:A:146:ASP:HB3  | 1:A:76:SER:HA    | 3        | 0.33          |
| (1,825) | 1:A:146:ASP:HB2  | 1:A:76:SER:HA    | 7        | 0.33          |
| (1,824) | 1:A:146:ASP:HB2  | 1:A:76:SER:HA    | 7        | 0.33          |
| (1,817) | 1:A:145:VAL:HB   | 1:A:145:VAL:H    | 2        | 0.33          |
| (1,811) | 1:A:145:VAL:HB   | 1:A:77:VAL:HB    | 7        | 0.33          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG11 | 4        | 0.33          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG12 | 4        | 0.33          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG13 | 4        | 0.33          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG21 | 4        | 0.33          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG22 | 4        | 0.33          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG23 | 4        | 0.33          |
| (1,742) | 1:A:135:SER:HA   | 1:A:145:VAL:HA   | 3        | 0.33          |
| (1,742) | 1:A:135:SER:HA   | 1:A:145:VAL:HA   | 6        | 0.33          |
| (1,740) | 1:A:135:SER:HA   | 1:A:145:VAL:HA   | 3        | 0.33          |
| (1,740) | 1:A:135:SER:HA   | 1:A:145:VAL:HA   | 6        | 0.33          |
| (1,729) | 1:A:134:THR:H    | 1:A:134:THR:HG21 | 9        | 0.33          |
| (1,729) | 1:A:134:THR:H    | 1:A:134:THR:HG22 | 9        | 0.33          |
| (1,729) | 1:A:134:THR:H    | 1:A:134:THR:HG23 | 9        | 0.33          |
| (1,719) | 1:A:133:ILE:HG21 | 1:A:133:ILE:HA   | 1        | 0.33          |
| (1,719) | 1:A:133:ILE:HG22 | 1:A:133:ILE:HA   | 1        | 0.33          |
| (1,719) | 1:A:133:ILE:HG23 | 1:A:133:ILE:HA   | 1        | 0.33          |
| (1,682) | 1:A:129:ASP:H    | 1:A:128:VAL:HA   | 1        | 0.33          |
| (1,680) | 1:A:128:VAL:H    | 1:A:129:ASP:H    | 8        | 0.33          |
| (1,650) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HB   | 5        | 0.33          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,621) | 1:A:124:ILE:HD11 | 1:A:123:ARG:HA  | 6        | 0.33          |
| (1,621) | 1:A:124:ILE:HD12 | 1:A:123:ARG:HA  | 6        | 0.33          |
| (1,621) | 1:A:124:ILE:HD13 | 1:A:123:ARG:HA  | 6        | 0.33          |
| (1,621) | 1:A:124:ILE:HD11 | 1:A:123:ARG:HA  | 8        | 0.33          |
| (1,621) | 1:A:124:ILE:HD12 | 1:A:123:ARG:HA  | 8        | 0.33          |
| (1,621) | 1:A:124:ILE:HD13 | 1:A:123:ARG:HA  | 8        | 0.33          |
| (1,609) | 1:A:123:ARG:HA   | 1:A:123:ARG:HD2 | 6        | 0.33          |
| (1,609) | 1:A:123:ARG:HA   | 1:A:123:ARG:HD3 | 6        | 0.33          |
| (1,539) | 1:A:116:ARG:H    | 1:A:116:ARG:HG2 | 1        | 0.33          |
| (1,539) | 1:A:116:ARG:H    | 1:A:116:ARG:HG3 | 1        | 0.33          |
| (1,518) | 1:A:114:ILE:HG21 | 1:A:114:ILE:H   | 2        | 0.33          |
| (1,518) | 1:A:114:ILE:HG22 | 1:A:114:ILE:H   | 2        | 0.33          |
| (1,518) | 1:A:114:ILE:HG23 | 1:A:114:ILE:H   | 2        | 0.33          |
| (1,518) | 1:A:114:ILE:HG21 | 1:A:114:ILE:H   | 6        | 0.33          |
| (1,518) | 1:A:114:ILE:HG22 | 1:A:114:ILE:H   | 6        | 0.33          |
| (1,518) | 1:A:114:ILE:HG23 | 1:A:114:ILE:H   | 6        | 0.33          |
| (1,5)   | 1:A:67:GLU:H     | 1:A:67:GLU:HA   | 4        | 0.33          |
| (1,5)   | 1:A:67:GLU:H     | 1:A:67:GLU:HA   | 5        | 0.33          |
| (1,494) | 1:A:113:PHE:HA   | 1:A:113:PHE:HD1 | 9        | 0.33          |
| (1,494) | 1:A:113:PHE:HA   | 1:A:113:PHE:HD2 | 9        | 0.33          |
| (1,485) | 1:A:113:PHE:HA   | 1:A:108:GLN:HA  | 2        | 0.33          |
| (1,468) | 1:A:111:HIS:H    | 1:A:112:GLY:H   | 1        | 0.33          |
| (1,411) | 1:A:105:GLU:HB2  | 1:A:105:GLU:H   | 8        | 0.33          |
| (1,411) | 1:A:105:GLU:HB3  | 1:A:105:GLU:H   | 8        | 0.33          |
| (1,408) | 1:A:104:HIS:HB3  | 1:A:105:GLU:H   | 3        | 0.33          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD11 | 4        | 0.33          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD12 | 4        | 0.33          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD13 | 4        | 0.33          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD21 | 4        | 0.33          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD22 | 4        | 0.33          |
| (1,4)   | 1:A:66:SER:HA    | 1:A:79:LEU:HD23 | 4        | 0.33          |
| (1,287) | 1:A:93:VAL:HA    | 1:A:98:ILE:HA   | 6        | 0.33          |
| (1,285) | 1:A:93:VAL:HG11  | 1:A:93:VAL:H    | 3        | 0.33          |
| (1,285) | 1:A:93:VAL:HG12  | 1:A:93:VAL:H    | 3        | 0.33          |
| (1,285) | 1:A:93:VAL:HG13  | 1:A:93:VAL:H    | 3        | 0.33          |
| (1,285) | 1:A:93:VAL:HG21  | 1:A:93:VAL:H    | 3        | 0.33          |
| (1,285) | 1:A:93:VAL:HG22  | 1:A:93:VAL:H    | 3        | 0.33          |
| (1,285) | 1:A:93:VAL:HG23  | 1:A:93:VAL:H    | 3        | 0.33          |
| (1,253) | 1:A:89:LEU:HA    | 1:A:90:LYS:H    | 6        | 0.33          |
| (1,253) | 1:A:89:LEU:HA    | 1:A:90:LYS:H    | 8        | 0.33          |
| (1,231) | 1:A:87:GLU:HB2   | 1:A:89:LEU:H    | 9        | 0.33          |
| (1,231) | 1:A:87:GLU:HB3   | 1:A:89:LEU:H    | 9        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,218)  | 1:A:86:PRO:HB2   | 1:A:85:SER:HA    | 7        | 0.33          |
| (1,218)  | 1:A:86:PRO:HB3   | 1:A:85:SER:HA    | 7        | 0.33          |
| (1,195)  | 1:A:84:PHE:HD1   | 1:A:84:PHE:H     | 5        | 0.33          |
| (1,195)  | 1:A:84:PHE:HD2   | 1:A:84:PHE:H     | 5        | 0.33          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE1  | 4        | 0.33          |
| (1,1742) | 1:A:114:ILE:HG21 | 1:B:118:PHE:HE2  | 4        | 0.33          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE1  | 4        | 0.33          |
| (1,1742) | 1:A:114:ILE:HG22 | 1:B:118:PHE:HE2  | 4        | 0.33          |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE1  | 4        | 0.33          |
| (1,1742) | 1:A:114:ILE:HG23 | 1:B:118:PHE:HE2  | 4        | 0.33          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD2  | 4        | 0.33          |
| (1,1724) | 1:B:150:LYS:H    | 1:B:150:LYS:HD3  | 4        | 0.33          |
| (1,1705) | 1:B:146:ASP:HB3  | 1:B:146:ASP:H    | 6        | 0.33          |
| (1,1694) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA    | 3        | 0.33          |
| (1,1693) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA    | 3        | 0.33          |
| (1,1692) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA    | 7        | 0.33          |
| (1,1691) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA    | 7        | 0.33          |
| (1,1684) | 1:B:145:VAL:HB   | 1:B:145:VAL:H    | 2        | 0.33          |
| (1,1678) | 1:B:145:VAL:HB   | 1:B:77:VAL:HB    | 7        | 0.33          |
| (1,1650) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1650) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1650) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1650) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1650) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1650) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1649) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1649) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1649) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1649) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1649) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1649) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H    | 4        | 0.33          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG11 | 6        | 0.33          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG12 | 6        | 0.33          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG13 | 6        | 0.33          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG21 | 6        | 0.33          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG22 | 6        | 0.33          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG23 | 6        | 0.33          |
| (1,1609) | 1:B:135:SER:HA   | 1:B:145:VAL:HA   | 3        | 0.33          |
| (1,1609) | 1:B:135:SER:HA   | 1:B:145:VAL:HA   | 6        | 0.33          |
| (1,1607) | 1:B:135:SER:HA   | 1:B:145:VAL:HA   | 3        | 0.33          |
| (1,1607) | 1:B:135:SER:HA   | 1:B:145:VAL:HA   | 6        | 0.33          |
| (1,1586) | 1:B:133:ILE:HG21 | 1:B:133:ILE:HA   | 1        | 0.33          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1586) | 1:B:133:ILE:HG22 | 1:B:133:ILE:HA  | 1        | 0.33          |
| (1,1586) | 1:B:133:ILE:HG23 | 1:B:133:ILE:HA  | 1        | 0.33          |
| (1,1549) | 1:B:129:ASP:H    | 1:B:128:VAL:HA  | 1        | 0.33          |
| (1,1547) | 1:B:128:VAL:H    | 1:B:129:ASP:H   | 8        | 0.33          |
| (1,1517) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HB  | 5        | 0.33          |
| (1,1517) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HB  | 6        | 0.33          |
| (1,1488) | 1:B:124:ILE:HD11 | 1:B:123:ARG:HA  | 6        | 0.33          |
| (1,1488) | 1:B:124:ILE:HD12 | 1:B:123:ARG:HA  | 6        | 0.33          |
| (1,1488) | 1:B:124:ILE:HD13 | 1:B:123:ARG:HA  | 6        | 0.33          |
| (1,1488) | 1:B:124:ILE:HD11 | 1:B:123:ARG:HA  | 8        | 0.33          |
| (1,1488) | 1:B:124:ILE:HD12 | 1:B:123:ARG:HA  | 8        | 0.33          |
| (1,1488) | 1:B:124:ILE:HD13 | 1:B:123:ARG:HA  | 8        | 0.33          |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG2 | 1        | 0.33          |
| (1,1406) | 1:B:116:ARG:H    | 1:B:116:ARG:HG3 | 1        | 0.33          |
| (1,1385) | 1:B:114:ILE:HG21 | 1:B:114:ILE:H   | 2        | 0.33          |
| (1,1385) | 1:B:114:ILE:HG22 | 1:B:114:ILE:H   | 2        | 0.33          |
| (1,1385) | 1:B:114:ILE:HG23 | 1:B:114:ILE:H   | 2        | 0.33          |
| (1,1385) | 1:B:114:ILE:HG21 | 1:B:114:ILE:H   | 6        | 0.33          |
| (1,1385) | 1:B:114:ILE:HG22 | 1:B:114:ILE:H   | 6        | 0.33          |
| (1,1385) | 1:B:114:ILE:HG23 | 1:B:114:ILE:H   | 6        | 0.33          |
| (1,1361) | 1:B:113:PHE:HA   | 1:B:113:PHE:HD1 | 9        | 0.33          |
| (1,1361) | 1:B:113:PHE:HA   | 1:B:113:PHE:HD2 | 9        | 0.33          |
| (1,1352) | 1:B:113:PHE:HA   | 1:B:108:GLN:HA  | 2        | 0.33          |
| (1,1335) | 1:B:111:HIS:H    | 1:B:112:GLY:H   | 1        | 0.33          |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE1 | 6        | 0.33          |
| (1,13)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HE2 | 6        | 0.33          |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE1 | 6        | 0.33          |
| (1,13)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HE2 | 6        | 0.33          |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE1 | 6        | 0.33          |
| (1,13)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HE2 | 6        | 0.33          |
| (1,128)  | 1:A:78:ASN:HA    | 1:A:79:LEU:H    | 2        | 0.33          |
| (1,1278) | 1:B:105:GLU:HB2  | 1:B:105:GLU:H   | 8        | 0.33          |
| (1,1278) | 1:B:105:GLU:HB3  | 1:B:105:GLU:H   | 8        | 0.33          |
| (1,1275) | 1:B:104:HIS:HB3  | 1:B:105:GLU:H   | 3        | 0.33          |
| (1,1244) | 1:B:101:HIS:HB3  | 1:B:101:HIS:HA  | 2        | 0.33          |
| (1,1240) | 1:B:101:HIS:HB3  | 1:B:101:HIS:HA  | 2        | 0.33          |
| (1,1154) | 1:B:93:VAL:HA    | 1:B:98:ILE:HA   | 6        | 0.33          |
| (1,1152) | 1:B:93:VAL:HG11  | 1:B:93:VAL:H    | 3        | 0.33          |
| (1,1152) | 1:B:93:VAL:HG12  | 1:B:93:VAL:H    | 3        | 0.33          |
| (1,1152) | 1:B:93:VAL:HG13  | 1:B:93:VAL:H    | 3        | 0.33          |
| (1,1152) | 1:B:93:VAL:HG21  | 1:B:93:VAL:H    | 3        | 0.33          |
| (1,1152) | 1:B:93:VAL:HG22  | 1:B:93:VAL:H    | 3        | 0.33          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1152) | 1:B:93:VAL:HG23 | 1:B:93:VAL:H   | 3        | 0.33          |
| (1,1152) | 1:B:93:VAL:HG11 | 1:B:93:VAL:H   | 4        | 0.33          |
| (1,1152) | 1:B:93:VAL:HG12 | 1:B:93:VAL:H   | 4        | 0.33          |
| (1,1152) | 1:B:93:VAL:HG13 | 1:B:93:VAL:H   | 4        | 0.33          |
| (1,1152) | 1:B:93:VAL:HG21 | 1:B:93:VAL:H   | 4        | 0.33          |
| (1,1152) | 1:B:93:VAL:HG22 | 1:B:93:VAL:H   | 4        | 0.33          |
| (1,1152) | 1:B:93:VAL:HG23 | 1:B:93:VAL:H   | 4        | 0.33          |
| (1,1147) | 1:B:92:LYS:H    | 1:B:100:VAL:HA | 1        | 0.33          |
| (1,1120) | 1:B:89:LEU:HA   | 1:B:90:LYS:H   | 6        | 0.33          |
| (1,1120) | 1:B:89:LEU:HA   | 1:B:90:LYS:H   | 8        | 0.33          |
| (1,1098) | 1:B:87:GLU:HB2  | 1:B:89:LEU:H   | 9        | 0.33          |
| (1,1098) | 1:B:87:GLU:HB3  | 1:B:89:LEU:H   | 9        | 0.33          |
| (1,1093) | 1:B:87:GLU:HG2  | 1:B:88:GLU:H   | 8        | 0.33          |
| (1,1093) | 1:B:87:GLU:HG3  | 1:B:88:GLU:H   | 8        | 0.33          |
| (1,1085) | 1:B:86:PRO:HB2  | 1:B:85:SER:HA  | 7        | 0.33          |
| (1,1085) | 1:B:86:PRO:HB3  | 1:B:85:SER:HA  | 7        | 0.33          |
| (1,997)  | 1:B:78:ASN:HB2  | 1:B:79:LEU:H   | 4        | 0.32          |
| (1,995)  | 1:B:78:ASN:HA   | 1:B:79:LEU:H   | 8        | 0.32          |
| (1,948)  | 1:B:77:VAL:HG11 | 1:B:68:MET:HE1 | 4        | 0.32          |
| (1,948)  | 1:B:77:VAL:HG11 | 1:B:68:MET:HE2 | 4        | 0.32          |
| (1,948)  | 1:B:77:VAL:HG11 | 1:B:68:MET:HE3 | 4        | 0.32          |
| (1,948)  | 1:B:77:VAL:HG12 | 1:B:68:MET:HE1 | 4        | 0.32          |
| (1,948)  | 1:B:77:VAL:HG12 | 1:B:68:MET:HE2 | 4        | 0.32          |
| (1,948)  | 1:B:77:VAL:HG12 | 1:B:68:MET:HE3 | 4        | 0.32          |
| (1,948)  | 1:B:77:VAL:HG13 | 1:B:68:MET:HE1 | 4        | 0.32          |
| (1,948)  | 1:B:77:VAL:HG13 | 1:B:68:MET:HE2 | 4        | 0.32          |
| (1,948)  | 1:B:77:VAL:HG13 | 1:B:68:MET:HE3 | 4        | 0.32          |
| (1,888)  | 1:B:70:LEU:HD11 | 1:B:71:GLU:H   | 5        | 0.32          |
| (1,888)  | 1:B:70:LEU:HD12 | 1:B:71:GLU:H   | 5        | 0.32          |
| (1,888)  | 1:B:70:LEU:HD13 | 1:B:71:GLU:H   | 5        | 0.32          |
| (1,888)  | 1:B:70:LEU:HD21 | 1:B:71:GLU:H   | 5        | 0.32          |
| (1,888)  | 1:B:70:LEU:HD22 | 1:B:71:GLU:H   | 5        | 0.32          |
| (1,888)  | 1:B:70:LEU:HD23 | 1:B:71:GLU:H   | 5        | 0.32          |
| (1,878)  | 1:B:68:MET:HG2  | 1:B:69:ARG:H   | 1        | 0.32          |
| (1,878)  | 1:B:68:MET:HG3  | 1:B:69:ARG:H   | 1        | 0.32          |
| (1,81)   | 1:A:77:VAL:HG11 | 1:A:68:MET:HE1 | 4        | 0.32          |
| (1,81)   | 1:A:77:VAL:HG11 | 1:A:68:MET:HE2 | 4        | 0.32          |
| (1,81)   | 1:A:77:VAL:HG11 | 1:A:68:MET:HE3 | 4        | 0.32          |
| (1,81)   | 1:A:77:VAL:HG12 | 1:A:68:MET:HE1 | 4        | 0.32          |
| (1,81)   | 1:A:77:VAL:HG12 | 1:A:68:MET:HE2 | 4        | 0.32          |
| (1,81)   | 1:A:77:VAL:HG12 | 1:A:68:MET:HE3 | 4        | 0.32          |
| (1,81)   | 1:A:77:VAL:HG13 | 1:A:68:MET:HE1 | 4        | 0.32          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,81)  | 1:A:77:VAL:HG13  | 1:A:68:MET:HE2   | 4        | 0.32          |
| (1,81)  | 1:A:77:VAL:HG13  | 1:A:68:MET:HE3   | 4        | 0.32          |
| (1,809) | 1:A:144:THR:HG21 | 1:A:146:ASP:HB3  | 7        | 0.32          |
| (1,809) | 1:A:144:THR:HG22 | 1:A:146:ASP:HB3  | 7        | 0.32          |
| (1,809) | 1:A:144:THR:HG23 | 1:A:146:ASP:HB3  | 7        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG11 | 6        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG12 | 6        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG13 | 6        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG21 | 6        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG22 | 6        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG23 | 6        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG11 | 9        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG12 | 9        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG13 | 9        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG21 | 9        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG22 | 9        | 0.32          |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG23 | 9        | 0.32          |
| (1,727) | 1:A:133:ILE:HG21 | 1:A:145:VAL:HB   | 2        | 0.32          |
| (1,727) | 1:A:133:ILE:HG22 | 1:A:145:VAL:HB   | 2        | 0.32          |
| (1,727) | 1:A:133:ILE:HG23 | 1:A:145:VAL:HB   | 2        | 0.32          |
| (1,682) | 1:A:129:ASP:H    | 1:A:128:VAL:HA   | 6        | 0.32          |
| (1,682) | 1:A:129:ASP:H    | 1:A:128:VAL:HA   | 7        | 0.32          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG11 | 7        | 0.32          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG12 | 7        | 0.32          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG13 | 7        | 0.32          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG21 | 7        | 0.32          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG22 | 7        | 0.32          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG23 | 7        | 0.32          |
| (1,650) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HB   | 6        | 0.32          |
| (1,650) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HB   | 9        | 0.32          |
| (1,621) | 1:A:124:ILE:HD11 | 1:A:123:ARG:HA   | 3        | 0.32          |
| (1,621) | 1:A:124:ILE:HD12 | 1:A:123:ARG:HA   | 3        | 0.32          |
| (1,621) | 1:A:124:ILE:HD13 | 1:A:123:ARG:HA   | 3        | 0.32          |
| (1,578) | 1:A:119:HIS:HA   | 1:A:119:HIS:H    | 1        | 0.32          |
| (1,574) | 1:A:119:HIS:HB3  | 1:A:119:HIS:HD2  | 3        | 0.32          |
| (1,546) | 1:A:117:GLU:HA   | 1:A:117:GLU:H    | 3        | 0.32          |
| (1,511) | 1:A:114:ILE:HG21 | 1:A:112:GLY:H    | 8        | 0.32          |
| (1,511) | 1:A:114:ILE:HG22 | 1:A:112:GLY:H    | 8        | 0.32          |
| (1,511) | 1:A:114:ILE:HG23 | 1:A:112:GLY:H    | 8        | 0.32          |
| (1,445) | 1:A:108:GLN:HA   | 1:A:113:PHE:H    | 2        | 0.32          |
| (1,421) | 1:A:107:ARG:HD2  | 1:A:105:GLU:H    | 3        | 0.32          |
| (1,378) | 1:A:101:HIS:HB3  | 1:A:101:HIS:H    | 5        | 0.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,377)  | 1:A:101:HIS:HB3 | 1:A:101:HIS:HA  | 2        | 0.32          |
| (1,373)  | 1:A:101:HIS:HB3 | 1:A:101:HIS:HA  | 2        | 0.32          |
| (1,351)  | 1:A:99:GLU:HA   | 1:A:99:GLU:H    | 8        | 0.32          |
| (1,337)  | 1:A:98:ILE:HD11 | 1:A:98:ILE:HB   | 1        | 0.32          |
| (1,337)  | 1:A:98:ILE:HD12 | 1:A:98:ILE:HB   | 1        | 0.32          |
| (1,337)  | 1:A:98:ILE:HD13 | 1:A:98:ILE:HB   | 1        | 0.32          |
| (1,337)  | 1:A:98:ILE:HD11 | 1:A:98:ILE:HB   | 2        | 0.32          |
| (1,337)  | 1:A:98:ILE:HD12 | 1:A:98:ILE:HB   | 2        | 0.32          |
| (1,337)  | 1:A:98:ILE:HD13 | 1:A:98:ILE:HB   | 2        | 0.32          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG11 | 7        | 0.32          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG12 | 7        | 0.32          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG13 | 7        | 0.32          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG21 | 7        | 0.32          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG22 | 7        | 0.32          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG23 | 7        | 0.32          |
| (1,306)  | 1:A:95:GLY:HA2  | 1:A:97:VAL:H    | 2        | 0.32          |
| (1,305)  | 1:A:95:GLY:HA2  | 1:A:96:ASP:H    | 3        | 0.32          |
| (1,291)  | 1:A:94:LEU:HD11 | 1:A:94:LEU:H    | 2        | 0.32          |
| (1,291)  | 1:A:94:LEU:HD12 | 1:A:94:LEU:H    | 2        | 0.32          |
| (1,291)  | 1:A:94:LEU:HD13 | 1:A:94:LEU:H    | 2        | 0.32          |
| (1,291)  | 1:A:94:LEU:HD21 | 1:A:94:LEU:H    | 2        | 0.32          |
| (1,291)  | 1:A:94:LEU:HD22 | 1:A:94:LEU:H    | 2        | 0.32          |
| (1,291)  | 1:A:94:LEU:HD23 | 1:A:94:LEU:H    | 2        | 0.32          |
| (1,285)  | 1:A:93:VAL:HG11 | 1:A:93:VAL:H    | 1        | 0.32          |
| (1,285)  | 1:A:93:VAL:HG12 | 1:A:93:VAL:H    | 1        | 0.32          |
| (1,285)  | 1:A:93:VAL:HG13 | 1:A:93:VAL:H    | 1        | 0.32          |
| (1,285)  | 1:A:93:VAL:HG21 | 1:A:93:VAL:H    | 1        | 0.32          |
| (1,285)  | 1:A:93:VAL:HG22 | 1:A:93:VAL:H    | 1        | 0.32          |
| (1,285)  | 1:A:93:VAL:HG23 | 1:A:93:VAL:H    | 1        | 0.32          |
| (1,280)  | 1:A:92:LYS:H    | 1:A:100:VAL:HA  | 1        | 0.32          |
| (1,253)  | 1:A:89:LEU:HA   | 1:A:90:LYS:H    | 7        | 0.32          |
| (1,226)  | 1:A:87:GLU:HG2  | 1:A:88:GLU:H    | 6        | 0.32          |
| (1,226)  | 1:A:87:GLU:HG3  | 1:A:88:GLU:H    | 6        | 0.32          |
| (1,218)  | 1:A:86:PRO:HB2  | 1:A:85:SER:HA   | 5        | 0.32          |
| (1,218)  | 1:A:86:PRO:HB3  | 1:A:85:SER:HA   | 5        | 0.32          |
| (1,21)   | 1:A:70:LEU:HD11 | 1:A:71:GLU:H    | 5        | 0.32          |
| (1,21)   | 1:A:70:LEU:HD12 | 1:A:71:GLU:H    | 5        | 0.32          |
| (1,21)   | 1:A:70:LEU:HD13 | 1:A:71:GLU:H    | 5        | 0.32          |
| (1,21)   | 1:A:70:LEU:HD21 | 1:A:71:GLU:H    | 5        | 0.32          |
| (1,21)   | 1:A:70:LEU:HD22 | 1:A:71:GLU:H    | 5        | 0.32          |
| (1,21)   | 1:A:70:LEU:HD23 | 1:A:71:GLU:H    | 5        | 0.32          |
| (1,1756) | 1:A:118:PHE:HA  | 1:B:117:GLU:H   | 3        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1676) | 1:B:144:THR:HG21 | 1:B:146:ASP:HB3  | 7        | 0.32          |
| (1,1676) | 1:B:144:THR:HG22 | 1:B:146:ASP:HB3  | 7        | 0.32          |
| (1,1676) | 1:B:144:THR:HG23 | 1:B:146:ASP:HB3  | 7        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG11 | 2        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG12 | 2        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG13 | 2        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG21 | 2        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG22 | 2        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG23 | 2        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG11 | 9        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG12 | 9        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG13 | 9        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG21 | 9        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG22 | 9        | 0.32          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG23 | 9        | 0.32          |
| (1,1549) | 1:B:129:ASP:H    | 1:B:128:VAL:HA   | 6        | 0.32          |
| (1,1549) | 1:B:129:ASP:H    | 1:B:128:VAL:HA   | 7        | 0.32          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG11 | 7        | 0.32          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG12 | 7        | 0.32          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG13 | 7        | 0.32          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG21 | 7        | 0.32          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG22 | 7        | 0.32          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG23 | 7        | 0.32          |
| (1,1517) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HB   | 9        | 0.32          |
| (1,1445) | 1:B:119:HIS:HA   | 1:B:119:HIS:H    | 1        | 0.32          |
| (1,1413) | 1:B:117:GLU:HA   | 1:B:117:GLU:H    | 3        | 0.32          |
| (1,1378) | 1:B:114:ILE:HG21 | 1:B:112:GLY:H    | 8        | 0.32          |
| (1,1378) | 1:B:114:ILE:HG22 | 1:B:112:GLY:H    | 8        | 0.32          |
| (1,1378) | 1:B:114:ILE:HG23 | 1:B:112:GLY:H    | 8        | 0.32          |
| (1,1312) | 1:B:108:GLN:HA   | 1:B:113:PHE:H    | 2        | 0.32          |
| (1,130)  | 1:A:78:ASN:HB2   | 1:A:79:LEU:H     | 4        | 0.32          |
| (1,1288) | 1:B:107:ARG:HD2  | 1:B:105:GLU:H    | 3        | 0.32          |
| (1,1282) | 1:B:105:GLU:HA   | 1:B:106:GLU:H    | 3        | 0.32          |
| (1,128)  | 1:A:78:ASN:HA    | 1:A:79:LEU:H     | 8        | 0.32          |
| (1,1245) | 1:B:101:HIS:HB3  | 1:B:101:HIS:H    | 5        | 0.32          |
| (1,1218) | 1:B:99:GLU:HA    | 1:B:99:GLU:H     | 8        | 0.32          |
| (1,1204) | 1:B:98:ILE:HD11  | 1:B:98:ILE:HB    | 1        | 0.32          |
| (1,1204) | 1:B:98:ILE:HD12  | 1:B:98:ILE:HB    | 1        | 0.32          |
| (1,1204) | 1:B:98:ILE:HD13  | 1:B:98:ILE:HB    | 1        | 0.32          |
| (1,1204) | 1:B:98:ILE:HD11  | 1:B:98:ILE:HB    | 2        | 0.32          |
| (1,1204) | 1:B:98:ILE:HD12  | 1:B:98:ILE:HB    | 2        | 0.32          |
| (1,1204) | 1:B:98:ILE:HD13  | 1:B:98:ILE:HB    | 2        | 0.32          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG11  | 7        | 0.32          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG12  | 7        | 0.32          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG13  | 7        | 0.32          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG21  | 7        | 0.32          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG22  | 7        | 0.32          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG23  | 7        | 0.32          |
| (1,1173) | 1:B:95:GLY:HA2  | 1:B:97:VAL:H     | 2        | 0.32          |
| (1,1172) | 1:B:95:GLY:HA2  | 1:B:96:ASP:H     | 3        | 0.32          |
| (1,1158) | 1:B:94:LEU:HD11 | 1:B:94:LEU:H     | 2        | 0.32          |
| (1,1158) | 1:B:94:LEU:HD12 | 1:B:94:LEU:H     | 2        | 0.32          |
| (1,1158) | 1:B:94:LEU:HD13 | 1:B:94:LEU:H     | 2        | 0.32          |
| (1,1158) | 1:B:94:LEU:HD21 | 1:B:94:LEU:H     | 2        | 0.32          |
| (1,1158) | 1:B:94:LEU:HD22 | 1:B:94:LEU:H     | 2        | 0.32          |
| (1,1158) | 1:B:94:LEU:HD23 | 1:B:94:LEU:H     | 2        | 0.32          |
| (1,1152) | 1:B:93:VAL:HG11 | 1:B:93:VAL:H     | 1        | 0.32          |
| (1,1152) | 1:B:93:VAL:HG12 | 1:B:93:VAL:H     | 1        | 0.32          |
| (1,1152) | 1:B:93:VAL:HG13 | 1:B:93:VAL:H     | 1        | 0.32          |
| (1,1152) | 1:B:93:VAL:HG21 | 1:B:93:VAL:H     | 1        | 0.32          |
| (1,1152) | 1:B:93:VAL:HG22 | 1:B:93:VAL:H     | 1        | 0.32          |
| (1,1152) | 1:B:93:VAL:HG23 | 1:B:93:VAL:H     | 1        | 0.32          |
| (1,1131) | 1:B:90:LYS:HG2  | 1:B:90:LYS:H     | 1        | 0.32          |
| (1,1131) | 1:B:90:LYS:HG3  | 1:B:90:LYS:H     | 1        | 0.32          |
| (1,1120) | 1:B:89:LEU:HA   | 1:B:90:LYS:H     | 7        | 0.32          |
| (1,11)   | 1:A:68:MET:HG2  | 1:A:69:ARG:H     | 1        | 0.32          |
| (1,11)   | 1:A:68:MET:HG3  | 1:A:69:ARG:H     | 1        | 0.32          |
| (1,1093) | 1:B:87:GLU:HG2  | 1:B:88:GLU:H     | 6        | 0.32          |
| (1,1093) | 1:B:87:GLU:HG3  | 1:B:88:GLU:H     | 6        | 0.32          |
| (1,1085) | 1:B:86:PRO:HB2  | 1:B:85:SER:HA    | 5        | 0.32          |
| (1,1085) | 1:B:86:PRO:HB3  | 1:B:85:SER:HA    | 5        | 0.32          |
| (1,1062) | 1:B:84:PHE:HD1  | 1:B:84:PHE:H     | 5        | 0.32          |
| (1,1062) | 1:B:84:PHE:HD2  | 1:B:84:PHE:H     | 5        | 0.32          |
| (1,980)  | 1:B:77:VAL:HB   | 1:B:145:VAL:HG21 | 9        | 0.31          |
| (1,980)  | 1:B:77:VAL:HB   | 1:B:145:VAL:HG22 | 9        | 0.31          |
| (1,980)  | 1:B:77:VAL:HB   | 1:B:145:VAL:HG23 | 9        | 0.31          |
| (1,954)  | 1:B:77:VAL:HG21 | 1:B:75:PHE:HD1   | 2        | 0.31          |
| (1,954)  | 1:B:77:VAL:HG21 | 1:B:75:PHE:HD2   | 2        | 0.31          |
| (1,954)  | 1:B:77:VAL:HG22 | 1:B:75:PHE:HD1   | 2        | 0.31          |
| (1,954)  | 1:B:77:VAL:HG22 | 1:B:75:PHE:HD2   | 2        | 0.31          |
| (1,954)  | 1:B:77:VAL:HG23 | 1:B:75:PHE:HD1   | 2        | 0.31          |
| (1,954)  | 1:B:77:VAL:HG23 | 1:B:75:PHE:HD2   | 2        | 0.31          |
| (1,915)  | 1:B:75:PHE:HA   | 1:B:75:PHE:HB3   | 2        | 0.31          |
| (1,909)  | 1:B:74:ARG:H    | 1:B:74:ARG:HB2   | 3        | 0.31          |

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| Key     | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,87)  | 1:A:77:VAL:HG21 | 1:A:75:PHE:HD1   | 2        | 0.31          |
| (1,87)  | 1:A:77:VAL:HG21 | 1:A:75:PHE:HD2   | 2        | 0.31          |
| (1,87)  | 1:A:77:VAL:HG22 | 1:A:75:PHE:HD1   | 2        | 0.31          |
| (1,87)  | 1:A:77:VAL:HG22 | 1:A:75:PHE:HD2   | 2        | 0.31          |
| (1,87)  | 1:A:77:VAL:HG23 | 1:A:75:PHE:HD1   | 2        | 0.31          |
| (1,87)  | 1:A:77:VAL:HG23 | 1:A:75:PHE:HD2   | 2        | 0.31          |
| (1,863) | 1:A:150:LYS:H   | 1:A:151:GLN:H    | 6        | 0.31          |
| (1,860) | 1:A:150:LYS:H   | 1:A:151:GLN:H    | 6        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG11 | 2        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG12 | 2        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG13 | 2        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG21 | 2        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG22 | 2        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG23 | 2        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG11 | 7        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG12 | 7        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG13 | 7        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG21 | 7        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG22 | 7        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG23 | 7        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG11 | 8        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG12 | 8        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG13 | 8        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG21 | 8        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG22 | 8        | 0.31          |
| (1,779) | 1:A:142:VAL:HA  | 1:A:142:VAL:HG23 | 8        | 0.31          |
| (1,778) | 1:A:142:VAL:H   | 1:A:141:GLY:H    | 4        | 0.31          |
| (1,777) | 1:A:142:VAL:H   | 1:A:141:GLY:H    | 4        | 0.31          |
| (1,770) | 1:A:141:GLY:H   | 1:A:140:ASP:H    | 2        | 0.31          |
| (1,768) | 1:A:141:GLY:H   | 1:A:140:ASP:H    | 2        | 0.31          |
| (1,742) | 1:A:135:SER:HA  | 1:A:145:VAL:HA   | 5        | 0.31          |
| (1,740) | 1:A:135:SER:HA  | 1:A:145:VAL:HA   | 5        | 0.31          |
| (1,682) | 1:A:129:ASP:H   | 1:A:128:VAL:HA   | 3        | 0.31          |
| (1,682) | 1:A:129:ASP:H   | 1:A:128:VAL:HA   | 5        | 0.31          |
| (1,682) | 1:A:129:ASP:H   | 1:A:128:VAL:HA   | 9        | 0.31          |
| (1,661) | 1:A:126:ALA:HB1 | 1:A:128:VAL:H    | 8        | 0.31          |
| (1,661) | 1:A:126:ALA:HB2 | 1:A:128:VAL:H    | 8        | 0.31          |
| (1,661) | 1:A:126:ALA:HB3 | 1:A:128:VAL:H    | 8        | 0.31          |
| (1,650) | 1:A:125:PRO:HD3 | 1:A:124:ILE:HB   | 1        | 0.31          |
| (1,585) | 1:A:121:LYS:HG2 | 1:A:121:LYS:HA   | 4        | 0.31          |
| (1,585) | 1:A:121:LYS:HG3 | 1:A:121:LYS:HA   | 4        | 0.31          |
| (1,578) | 1:A:119:HIS:HA  | 1:A:119:HIS:H    | 5        | 0.31          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,576) | 1:A:119:HIS:HB3  | 1:A:119:HIS:HA  | 5        | 0.31          |
| (1,575) | 1:A:119:HIS:HB3  | 1:A:119:HIS:HA  | 5        | 0.31          |
| (1,510) | 1:A:114:ILE:HG21 | 1:A:111:HIS:H   | 2        | 0.31          |
| (1,510) | 1:A:114:ILE:HG22 | 1:A:111:HIS:H   | 2        | 0.31          |
| (1,510) | 1:A:114:ILE:HG23 | 1:A:111:HIS:H   | 2        | 0.31          |
| (1,5)   | 1:A:67:GLU:H     | 1:A:67:GLU:HA   | 7        | 0.31          |
| (1,487) | 1:A:113:PHE:H    | 1:A:112:GLY:H   | 1        | 0.31          |
| (1,48)  | 1:A:75:PHE:HA    | 1:A:75:PHE:HB3  | 2        | 0.31          |
| (1,465) | 1:A:111:HIS:HB2  | 1:A:111:HIS:H   | 2        | 0.31          |
| (1,437) | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD1 | 2        | 0.31          |
| (1,437) | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD2 | 2        | 0.31          |
| (1,426) | 1:A:107:ARG:HD2  | 1:A:107:ARG:H   | 3        | 0.31          |
| (1,42)  | 1:A:74:ARG:H     | 1:A:74:ARG:HB2  | 3        | 0.31          |
| (1,415) | 1:A:105:GLU:HA   | 1:A:106:GLU:H   | 3        | 0.31          |
| (1,414) | 1:A:105:GLU:HG2  | 1:A:105:GLU:H   | 3        | 0.31          |
| (1,414) | 1:A:105:GLU:HG3  | 1:A:105:GLU:H   | 3        | 0.31          |
| (1,407) | 1:A:104:HIS:HA   | 1:A:105:GLU:H   | 7        | 0.31          |
| (1,337) | 1:A:98:ILE:HD11  | 1:A:98:ILE:HB   | 5        | 0.31          |
| (1,337) | 1:A:98:ILE:HD12  | 1:A:98:ILE:HB   | 5        | 0.31          |
| (1,337) | 1:A:98:ILE:HD13  | 1:A:98:ILE:HB   | 5        | 0.31          |
| (1,337) | 1:A:98:ILE:HD11  | 1:A:98:ILE:HB   | 6        | 0.31          |
| (1,337) | 1:A:98:ILE:HD12  | 1:A:98:ILE:HB   | 6        | 0.31          |
| (1,337) | 1:A:98:ILE:HD13  | 1:A:98:ILE:HB   | 6        | 0.31          |
| (1,314) | 1:A:96:ASP:HB2   | 1:A:96:ASP:H    | 5        | 0.31          |
| (1,314) | 1:A:96:ASP:HB3   | 1:A:96:ASP:H    | 5        | 0.31          |
| (1,313) | 1:A:96:ASP:HB2   | 1:A:96:ASP:H    | 5        | 0.31          |
| (1,313) | 1:A:96:ASP:HB3   | 1:A:96:ASP:H    | 5        | 0.31          |
| (1,311) | 1:A:96:ASP:HB2   | 1:A:96:ASP:H    | 5        | 0.31          |
| (1,311) | 1:A:96:ASP:HB3   | 1:A:96:ASP:H    | 5        | 0.31          |
| (1,306) | 1:A:95:GLY:HA2   | 1:A:97:VAL:H    | 4        | 0.31          |
| (1,306) | 1:A:95:GLY:HA2   | 1:A:97:VAL:H    | 8        | 0.31          |
| (1,287) | 1:A:93:VAL:HA    | 1:A:98:ILE:HA   | 3        | 0.31          |
| (1,281) | 1:A:92:LYS:H     | 1:A:101:HIS:H   | 9        | 0.31          |
| (1,264) | 1:A:90:LYS:HG2   | 1:A:90:LYS:H    | 1        | 0.31          |
| (1,264) | 1:A:90:LYS:HG3   | 1:A:90:LYS:H    | 1        | 0.31          |
| (1,245) | 1:A:89:LEU:HA    | 1:A:89:LEU:HD21 | 4        | 0.31          |
| (1,245) | 1:A:89:LEU:HA    | 1:A:89:LEU:HD22 | 4        | 0.31          |
| (1,245) | 1:A:89:LEU:HA    | 1:A:89:LEU:HD23 | 4        | 0.31          |
| (1,245) | 1:A:89:LEU:HA    | 1:A:89:LEU:HD21 | 5        | 0.31          |
| (1,245) | 1:A:89:LEU:HA    | 1:A:89:LEU:HD22 | 5        | 0.31          |
| (1,245) | 1:A:89:LEU:HA    | 1:A:89:LEU:HD23 | 5        | 0.31          |
| (1,238) | 1:A:89:LEU:HD11  | 1:A:85:SER:H    | 9        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,238)  | 1:A:89:LEU:HD12  | 1:A:85:SER:H     | 9        | 0.31          |
| (1,238)  | 1:A:89:LEU:HD13  | 1:A:85:SER:H     | 9        | 0.31          |
| (1,226)  | 1:A:87:GLU:HG2   | 1:A:88:GLU:H     | 3        | 0.31          |
| (1,226)  | 1:A:87:GLU:HG3   | 1:A:88:GLU:H     | 3        | 0.31          |
| (1,1730) | 1:B:150:LYS:H    | 1:B:151:GLN:H    | 6        | 0.31          |
| (1,1727) | 1:B:150:LYS:H    | 1:B:151:GLN:H    | 6        | 0.31          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG11 | 8        | 0.31          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG12 | 8        | 0.31          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG13 | 8        | 0.31          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG21 | 8        | 0.31          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG22 | 8        | 0.31          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG23 | 8        | 0.31          |
| (1,1645) | 1:B:142:VAL:H    | 1:B:141:GLY:H    | 4        | 0.31          |
| (1,1644) | 1:B:142:VAL:H    | 1:B:141:GLY:H    | 4        | 0.31          |
| (1,1637) | 1:B:141:GLY:H    | 1:B:140:ASP:H    | 2        | 0.31          |
| (1,1635) | 1:B:141:GLY:H    | 1:B:140:ASP:H    | 2        | 0.31          |
| (1,1609) | 1:B:135:SER:HA   | 1:B:145:VAL:HA   | 5        | 0.31          |
| (1,1607) | 1:B:135:SER:HA   | 1:B:145:VAL:HA   | 5        | 0.31          |
| (1,1594) | 1:B:133:ILE:HG21 | 1:B:145:VAL:HB   | 2        | 0.31          |
| (1,1594) | 1:B:133:ILE:HG22 | 1:B:145:VAL:HB   | 2        | 0.31          |
| (1,1594) | 1:B:133:ILE:HG23 | 1:B:145:VAL:HB   | 2        | 0.31          |
| (1,1549) | 1:B:129:ASP:H    | 1:B:128:VAL:HA   | 3        | 0.31          |
| (1,1549) | 1:B:129:ASP:H    | 1:B:128:VAL:HA   | 5        | 0.31          |
| (1,1549) | 1:B:129:ASP:H    | 1:B:128:VAL:HA   | 9        | 0.31          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG11 | 8        | 0.31          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG12 | 8        | 0.31          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG13 | 8        | 0.31          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG21 | 8        | 0.31          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG22 | 8        | 0.31          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG23 | 8        | 0.31          |
| (1,1528) | 1:B:126:ALA:HB1  | 1:B:128:VAL:H    | 8        | 0.31          |
| (1,1528) | 1:B:126:ALA:HB2  | 1:B:128:VAL:H    | 8        | 0.31          |
| (1,1528) | 1:B:126:ALA:HB3  | 1:B:128:VAL:H    | 8        | 0.31          |
| (1,1517) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HB   | 1        | 0.31          |
| (1,1502) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 2        | 0.31          |
| (1,1502) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 2        | 0.31          |
| (1,1502) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H    | 2        | 0.31          |
| (1,1501) | 1:B:124:ILE:HD11 | 1:B:124:ILE:H    | 2        | 0.31          |
| (1,1501) | 1:B:124:ILE:HD12 | 1:B:124:ILE:H    | 2        | 0.31          |
| (1,1501) | 1:B:124:ILE:HD13 | 1:B:124:ILE:H    | 2        | 0.31          |
| (1,150)  | 1:A:81:VAL:HG11  | 1:A:79:LEU:HB2   | 6        | 0.31          |
| (1,150)  | 1:A:81:VAL:HG11  | 1:A:79:LEU:HB3   | 6        | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,150)  | 1:A:81:VAL:HG12  | 1:A:79:LEU:HB2   | 6        | 0.31          |
| (1,150)  | 1:A:81:VAL:HG12  | 1:A:79:LEU:HB3   | 6        | 0.31          |
| (1,150)  | 1:A:81:VAL:HG13  | 1:A:79:LEU:HB2   | 6        | 0.31          |
| (1,150)  | 1:A:81:VAL:HG13  | 1:A:79:LEU:HB3   | 6        | 0.31          |
| (1,1488) | 1:B:124:ILE:HD11 | 1:B:123:ARG:HA   | 3        | 0.31          |
| (1,1488) | 1:B:124:ILE:HD12 | 1:B:123:ARG:HA   | 3        | 0.31          |
| (1,1488) | 1:B:124:ILE:HD13 | 1:B:123:ARG:HA   | 3        | 0.31          |
| (1,1479) | 1:B:123:ARG:HB3  | 1:B:124:ILE:H    | 1        | 0.31          |
| (1,1452) | 1:B:121:LYS:HG2  | 1:B:121:LYS:HA   | 4        | 0.31          |
| (1,1452) | 1:B:121:LYS:HG3  | 1:B:121:LYS:HA   | 4        | 0.31          |
| (1,1445) | 1:B:119:HIS:HA   | 1:B:119:HIS:H    | 5        | 0.31          |
| (1,1443) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA   | 5        | 0.31          |
| (1,1442) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA   | 5        | 0.31          |
| (1,1441) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HD2  | 1        | 0.31          |
| (1,1377) | 1:B:114:ILE:HG21 | 1:B:111:HIS:H    | 2        | 0.31          |
| (1,1377) | 1:B:114:ILE:HG22 | 1:B:111:HIS:H    | 2        | 0.31          |
| (1,1377) | 1:B:114:ILE:HG23 | 1:B:111:HIS:H    | 2        | 0.31          |
| (1,1354) | 1:B:113:PHE:H    | 1:B:112:GLY:H    | 1        | 0.31          |
| (1,1332) | 1:B:111:HIS:HB2  | 1:B:111:HIS:H    | 2        | 0.31          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD1  | 2        | 0.31          |
| (1,1304) | 1:B:107:ARG:HB2  | 1:B:113:PHE:HD2  | 2        | 0.31          |
| (1,1293) | 1:B:107:ARG:HD2  | 1:B:107:ARG:H    | 3        | 0.31          |
| (1,1274) | 1:B:104:HIS:HA   | 1:B:105:GLU:H    | 7        | 0.31          |
| (1,1204) | 1:B:98:ILE:HD11  | 1:B:98:ILE:HB    | 6        | 0.31          |
| (1,1204) | 1:B:98:ILE:HD12  | 1:B:98:ILE:HB    | 6        | 0.31          |
| (1,1204) | 1:B:98:ILE:HD13  | 1:B:98:ILE:HB    | 6        | 0.31          |
| (1,1181) | 1:B:96:ASP:HB2   | 1:B:96:ASP:H     | 5        | 0.31          |
| (1,1181) | 1:B:96:ASP:HB3   | 1:B:96:ASP:H     | 5        | 0.31          |
| (1,1180) | 1:B:96:ASP:HB2   | 1:B:96:ASP:H     | 5        | 0.31          |
| (1,1180) | 1:B:96:ASP:HB3   | 1:B:96:ASP:H     | 5        | 0.31          |
| (1,1178) | 1:B:96:ASP:HB2   | 1:B:96:ASP:H     | 5        | 0.31          |
| (1,1178) | 1:B:96:ASP:HB3   | 1:B:96:ASP:H     | 5        | 0.31          |
| (1,1173) | 1:B:95:GLY:HA2   | 1:B:97:VAL:H     | 4        | 0.31          |
| (1,1173) | 1:B:95:GLY:HA2   | 1:B:97:VAL:H     | 8        | 0.31          |
| (1,1154) | 1:B:93:VAL:HA    | 1:B:98:ILE:HA    | 3        | 0.31          |
| (1,1148) | 1:B:92:LYS:H     | 1:B:101:HIS:H    | 9        | 0.31          |
| (1,1134) | 1:B:90:LYS:HB2   | 1:B:101:HIS:HB3  | 3        | 0.31          |
| (1,1134) | 1:B:90:LYS:HB3   | 1:B:101:HIS:HB3  | 3        | 0.31          |
| (1,1113) | 1:A:77:VAL:HB    | 1:A:145:VAL:HG21 | 9        | 0.31          |
| (1,1113) | 1:A:77:VAL:HB    | 1:A:145:VAL:HG22 | 9        | 0.31          |
| (1,1113) | 1:A:77:VAL:HB    | 1:A:145:VAL:HG23 | 9        | 0.31          |
| (1,1112) | 1:B:89:LEU:HA    | 1:B:89:LEU:HD21  | 4        | 0.31          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD22  | 4        | 0.31          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD23  | 4        | 0.31          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD21  | 5        | 0.31          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD22  | 5        | 0.31          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD23  | 5        | 0.31          |
| (1,1105) | 1:B:89:LEU:HD11 | 1:B:85:SER:H     | 9        | 0.31          |
| (1,1105) | 1:B:89:LEU:HD12 | 1:B:85:SER:H     | 9        | 0.31          |
| (1,1105) | 1:B:89:LEU:HD13 | 1:B:85:SER:H     | 9        | 0.31          |
| (1,1093) | 1:B:87:GLU:HG2  | 1:B:88:GLU:H     | 3        | 0.31          |
| (1,1093) | 1:B:87:GLU:HG3  | 1:B:88:GLU:H     | 3        | 0.31          |
| (1,1017) | 1:B:81:VAL:HG11 | 1:B:79:LEU:HB2   | 6        | 0.31          |
| (1,1017) | 1:B:81:VAL:HG11 | 1:B:79:LEU:HB3   | 6        | 0.31          |
| (1,1017) | 1:B:81:VAL:HG12 | 1:B:79:LEU:HB2   | 6        | 0.31          |
| (1,1017) | 1:B:81:VAL:HG12 | 1:B:79:LEU:HB3   | 6        | 0.31          |
| (1,1017) | 1:B:81:VAL:HG13 | 1:B:79:LEU:HB2   | 6        | 0.31          |
| (1,1017) | 1:B:81:VAL:HG13 | 1:B:79:LEU:HB3   | 6        | 0.31          |
| (1,975)  | 1:B:77:VAL:HG11 | 1:B:79:LEU:H     | 5        | 0.3           |
| (1,975)  | 1:B:77:VAL:HG12 | 1:B:79:LEU:H     | 5        | 0.3           |
| (1,975)  | 1:B:77:VAL:HG13 | 1:B:79:LEU:H     | 5        | 0.3           |
| (1,945)  | 1:B:76:SER:HA   | 1:B:146:ASP:HA   | 5        | 0.3           |
| (1,941)  | 1:B:76:SER:HA   | 1:B:146:ASP:HA   | 5        | 0.3           |
| (1,932)  | 1:B:76:SER:HB2  | 1:B:144:THR:HG21 | 2        | 0.3           |
| (1,932)  | 1:B:76:SER:HB2  | 1:B:144:THR:HG22 | 2        | 0.3           |
| (1,932)  | 1:B:76:SER:HB2  | 1:B:144:THR:HG23 | 2        | 0.3           |
| (1,918)  | 1:B:75:PHE:HA   | 1:B:76:SER:H     | 1        | 0.3           |
| (1,918)  | 1:B:75:PHE:HA   | 1:B:76:SER:H     | 5        | 0.3           |
| (1,891)  | 1:B:71:GLU:H    | 1:B:69:ARG:HG2   | 8        | 0.3           |
| (1,891)  | 1:B:71:GLU:H    | 1:B:69:ARG:HG3   | 8        | 0.3           |
| (1,872)  | 1:B:67:GLU:H    | 1:B:67:GLU:HA    | 7        | 0.3           |
| (1,854)  | 1:A:148:PRO:HB2 | 1:A:149:ARG:H    | 8        | 0.3           |
| (1,854)  | 1:A:148:PRO:HB3 | 1:A:149:ARG:H    | 8        | 0.3           |
| (1,825)  | 1:A:146:ASP:HB2 | 1:A:76:SER:HA    | 5        | 0.3           |
| (1,824)  | 1:A:146:ASP:HB2 | 1:A:76:SER:HA    | 5        | 0.3           |
| (1,804)  | 1:A:144:THR:HA  | 1:A:145:VAL:H    | 2        | 0.3           |
| (1,78)   | 1:A:76:SER:HA   | 1:A:146:ASP:HA   | 5        | 0.3           |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG11 | 3        | 0.3           |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG12 | 3        | 0.3           |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG13 | 3        | 0.3           |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG21 | 3        | 0.3           |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG22 | 3        | 0.3           |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG23 | 3        | 0.3           |
| (1,779)  | 1:A:142:VAL:HA  | 1:A:142:VAL:HG11 | 5        | 0.3           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG12 | 5        | 0.3           |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG13 | 5        | 0.3           |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG21 | 5        | 0.3           |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG22 | 5        | 0.3           |
| (1,779) | 1:A:142:VAL:HA   | 1:A:142:VAL:HG23 | 5        | 0.3           |
| (1,770) | 1:A:141:GLY:H    | 1:A:140:ASP:H    | 5        | 0.3           |
| (1,768) | 1:A:141:GLY:H    | 1:A:140:ASP:H    | 5        | 0.3           |
| (1,763) | 1:A:138:SER:H    | 1:A:142:VAL:H    | 2        | 0.3           |
| (1,760) | 1:A:138:SER:H    | 1:A:142:VAL:H    | 2        | 0.3           |
| (1,745) | 1:A:136:SER:H    | 1:A:135:SER:H    | 2        | 0.3           |
| (1,74)  | 1:A:76:SER:HA    | 1:A:146:ASP:HA   | 5        | 0.3           |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG21 | 4        | 0.3           |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG22 | 4        | 0.3           |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG23 | 4        | 0.3           |
| (1,719) | 1:A:133:ILE:HG21 | 1:A:133:ILE:HA   | 7        | 0.3           |
| (1,719) | 1:A:133:ILE:HG22 | 1:A:133:ILE:HA   | 7        | 0.3           |
| (1,719) | 1:A:133:ILE:HG23 | 1:A:133:ILE:HA   | 7        | 0.3           |
| (1,717) | 1:A:133:ILE:HG21 | 1:A:132:THR:H    | 9        | 0.3           |
| (1,717) | 1:A:133:ILE:HG22 | 1:A:132:THR:H    | 9        | 0.3           |
| (1,717) | 1:A:133:ILE:HG23 | 1:A:132:THR:H    | 9        | 0.3           |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG11 | 8        | 0.3           |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG12 | 8        | 0.3           |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG13 | 8        | 0.3           |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG21 | 8        | 0.3           |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG22 | 8        | 0.3           |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG23 | 8        | 0.3           |
| (1,65)  | 1:A:76:SER:HB2   | 1:A:144:THR:HG21 | 2        | 0.3           |
| (1,65)  | 1:A:76:SER:HB2   | 1:A:144:THR:HG22 | 2        | 0.3           |
| (1,65)  | 1:A:76:SER:HB2   | 1:A:144:THR:HG23 | 2        | 0.3           |
| (1,635) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 2        | 0.3           |
| (1,635) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 2        | 0.3           |
| (1,635) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 2        | 0.3           |
| (1,634) | 1:A:124:ILE:HD11 | 1:A:124:ILE:H    | 2        | 0.3           |
| (1,634) | 1:A:124:ILE:HD12 | 1:A:124:ILE:H    | 2        | 0.3           |
| (1,634) | 1:A:124:ILE:HD13 | 1:A:124:ILE:H    | 2        | 0.3           |
| (1,612) | 1:A:123:ARG:HB3  | 1:A:124:ILE:H    | 1        | 0.3           |
| (1,588) | 1:A:122:TYR:HB2  | 1:A:98:ILE:HD11  | 7        | 0.3           |
| (1,588) | 1:A:122:TYR:HB2  | 1:A:98:ILE:HD12  | 7        | 0.3           |
| (1,588) | 1:A:122:TYR:HB2  | 1:A:98:ILE:HD13  | 7        | 0.3           |
| (1,588) | 1:A:122:TYR:HB3  | 1:A:98:ILE:HD11  | 7        | 0.3           |
| (1,588) | 1:A:122:TYR:HB3  | 1:A:98:ILE:HD12  | 7        | 0.3           |
| (1,588) | 1:A:122:TYR:HB3  | 1:A:98:ILE:HD13  | 7        | 0.3           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,51)   | 1:A:75:PHE:HA   | 1:A:76:SER:H     | 1        | 0.3           |
| (1,51)   | 1:A:75:PHE:HA   | 1:A:76:SER:H     | 5        | 0.3           |
| (1,426)  | 1:A:107:ARG:HD2 | 1:A:107:ARG:H    | 6        | 0.3           |
| (1,376)  | 1:A:101:HIS:HB2 | 1:A:101:HIS:HD2  | 8        | 0.3           |
| (1,337)  | 1:A:98:ILE:HD11 | 1:A:98:ILE:HB    | 4        | 0.3           |
| (1,337)  | 1:A:98:ILE:HD12 | 1:A:98:ILE:HB    | 4        | 0.3           |
| (1,337)  | 1:A:98:ILE:HD13 | 1:A:98:ILE:HB    | 4        | 0.3           |
| (1,331)  | 1:A:97:VAL:HA   | 1:A:123:ARG:HD2  | 1        | 0.3           |
| (1,331)  | 1:A:97:VAL:HA   | 1:A:123:ARG:HD3  | 1        | 0.3           |
| (1,314)  | 1:A:96:ASP:HB2  | 1:A:96:ASP:H     | 2        | 0.3           |
| (1,314)  | 1:A:96:ASP:HB3  | 1:A:96:ASP:H     | 2        | 0.3           |
| (1,313)  | 1:A:96:ASP:HB2  | 1:A:96:ASP:H     | 2        | 0.3           |
| (1,313)  | 1:A:96:ASP:HB3  | 1:A:96:ASP:H     | 2        | 0.3           |
| (1,311)  | 1:A:96:ASP:HB2  | 1:A:96:ASP:H     | 2        | 0.3           |
| (1,311)  | 1:A:96:ASP:HB3  | 1:A:96:ASP:H     | 2        | 0.3           |
| (1,306)  | 1:A:95:GLY:HA2  | 1:A:97:VAL:H     | 7        | 0.3           |
| (1,278)  | 1:A:92:LYS:H    | 1:A:93:VAL:H     | 1        | 0.3           |
| (1,278)  | 1:A:92:LYS:H    | 1:A:93:VAL:H     | 3        | 0.3           |
| (1,267)  | 1:A:90:LYS:HB2  | 1:A:101:HIS:HB3  | 3        | 0.3           |
| (1,267)  | 1:A:90:LYS:HB3  | 1:A:101:HIS:HB3  | 3        | 0.3           |
| (1,242)  | 1:A:89:LEU:H    | 1:A:88:GLU:H     | 2        | 0.3           |
| (1,241)  | 1:A:89:LEU:H    | 1:A:88:GLU:H     | 2        | 0.3           |
| (1,24)   | 1:A:71:GLU:H    | 1:A:69:ARG:HG2   | 8        | 0.3           |
| (1,24)   | 1:A:71:GLU:H    | 1:A:69:ARG:HG3   | 8        | 0.3           |
| (1,226)  | 1:A:87:GLU:HG2  | 1:A:88:GLU:H     | 2        | 0.3           |
| (1,226)  | 1:A:87:GLU:HG3  | 1:A:88:GLU:H     | 2        | 0.3           |
| (1,201)  | 1:A:84:PHE:HD1  | 1:A:89:LEU:HA    | 1        | 0.3           |
| (1,201)  | 1:A:84:PHE:HD2  | 1:A:89:LEU:HA    | 1        | 0.3           |
| (1,182)  | 1:A:83:HIS:HA   | 1:A:84:PHE:H     | 4        | 0.3           |
| (1,181)  | 1:A:83:HIS:HB2  | 1:A:84:PHE:HB2   | 2        | 0.3           |
| (1,181)  | 1:A:83:HIS:HB2  | 1:A:84:PHE:HB3   | 2        | 0.3           |
| (1,175)  | 1:A:83:HIS:HA   | 1:A:83:HIS:HB3   | 2        | 0.3           |
| (1,174)  | 1:A:83:HIS:HA   | 1:A:83:HIS:HB3   | 2        | 0.3           |
| (1,1721) | 1:B:148:PRO:HB2 | 1:B:149:ARG:H    | 8        | 0.3           |
| (1,1721) | 1:B:148:PRO:HB3 | 1:B:149:ARG:H    | 8        | 0.3           |
| (1,1692) | 1:B:146:ASP:HB2 | 1:B:76:SER:HA    | 5        | 0.3           |
| (1,1691) | 1:B:146:ASP:HB2 | 1:B:76:SER:HA    | 5        | 0.3           |
| (1,1646) | 1:B:142:VAL:HA  | 1:B:142:VAL:HG11 | 3        | 0.3           |
| (1,1646) | 1:B:142:VAL:HA  | 1:B:142:VAL:HG12 | 3        | 0.3           |
| (1,1646) | 1:B:142:VAL:HA  | 1:B:142:VAL:HG13 | 3        | 0.3           |
| (1,1646) | 1:B:142:VAL:HA  | 1:B:142:VAL:HG21 | 3        | 0.3           |
| (1,1646) | 1:B:142:VAL:HA  | 1:B:142:VAL:HG22 | 3        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG23 | 3        | 0.3           |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG11 | 5        | 0.3           |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG12 | 5        | 0.3           |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG13 | 5        | 0.3           |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG21 | 5        | 0.3           |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG22 | 5        | 0.3           |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG23 | 5        | 0.3           |
| (1,1637) | 1:B:141:GLY:H    | 1:B:140:ASP:H    | 5        | 0.3           |
| (1,1635) | 1:B:141:GLY:H    | 1:B:140:ASP:H    | 5        | 0.3           |
| (1,1630) | 1:B:138:SER:H    | 1:B:142:VAL:H    | 2        | 0.3           |
| (1,163)  | 1:A:81:VAL:HG21  | 1:A:83:HIS:H     | 2        | 0.3           |
| (1,163)  | 1:A:81:VAL:HG22  | 1:A:83:HIS:H     | 2        | 0.3           |
| (1,163)  | 1:A:81:VAL:HG23  | 1:A:83:HIS:H     | 2        | 0.3           |
| (1,1627) | 1:B:138:SER:H    | 1:B:142:VAL:H    | 2        | 0.3           |
| (1,1612) | 1:B:136:SER:H    | 1:B:135:SER:H    | 2        | 0.3           |
| (1,1596) | 1:B:134:THR:H    | 1:B:134:THR:HG21 | 9        | 0.3           |
| (1,1596) | 1:B:134:THR:H    | 1:B:134:THR:HG22 | 9        | 0.3           |
| (1,1596) | 1:B:134:THR:H    | 1:B:134:THR:HG23 | 9        | 0.3           |
| (1,1586) | 1:B:133:ILE:HG21 | 1:B:133:ILE:HA   | 7        | 0.3           |
| (1,1586) | 1:B:133:ILE:HG22 | 1:B:133:ILE:HA   | 7        | 0.3           |
| (1,1586) | 1:B:133:ILE:HG23 | 1:B:133:ILE:HA   | 7        | 0.3           |
| (1,1584) | 1:B:133:ILE:HG21 | 1:B:132:THR:H    | 9        | 0.3           |
| (1,1584) | 1:B:133:ILE:HG22 | 1:B:132:THR:H    | 9        | 0.3           |
| (1,1584) | 1:B:133:ILE:HG23 | 1:B:132:THR:H    | 9        | 0.3           |
| (1,1517) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HB   | 2        | 0.3           |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD11  | 7        | 0.3           |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD12  | 7        | 0.3           |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD13  | 7        | 0.3           |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD11  | 7        | 0.3           |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD12  | 7        | 0.3           |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD13  | 7        | 0.3           |
| (1,1441) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HD2  | 6        | 0.3           |
| (1,1385) | 1:B:114:ILE:HG21 | 1:B:114:ILE:H    | 5        | 0.3           |
| (1,1385) | 1:B:114:ILE:HG22 | 1:B:114:ILE:H    | 5        | 0.3           |
| (1,1385) | 1:B:114:ILE:HG23 | 1:B:114:ILE:H    | 5        | 0.3           |
| (1,138)  | 1:A:79:LEU:HD11  | 1:A:79:LEU:HA    | 6        | 0.3           |
| (1,138)  | 1:A:79:LEU:HD12  | 1:A:79:LEU:HA    | 6        | 0.3           |
| (1,138)  | 1:A:79:LEU:HD13  | 1:A:79:LEU:HA    | 6        | 0.3           |
| (1,138)  | 1:A:79:LEU:HD21  | 1:A:79:LEU:HA    | 6        | 0.3           |
| (1,138)  | 1:A:79:LEU:HD22  | 1:A:79:LEU:HA    | 6        | 0.3           |
| (1,138)  | 1:A:79:LEU:HD23  | 1:A:79:LEU:HA    | 6        | 0.3           |
| (1,138)  | 1:A:79:LEU:HD11  | 1:A:79:LEU:HA    | 8        | 0.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,138)  | 1:A:79:LEU:HD12 | 1:A:79:LEU:HA   | 8        | 0.3           |
| (1,138)  | 1:A:79:LEU:HD13 | 1:A:79:LEU:HA   | 8        | 0.3           |
| (1,138)  | 1:A:79:LEU:HD21 | 1:A:79:LEU:HA   | 8        | 0.3           |
| (1,138)  | 1:A:79:LEU:HD22 | 1:A:79:LEU:HA   | 8        | 0.3           |
| (1,138)  | 1:A:79:LEU:HD23 | 1:A:79:LEU:HA   | 8        | 0.3           |
| (1,1293) | 1:B:107:ARG:HD2 | 1:B:107:ARG:H   | 6        | 0.3           |
| (1,1281) | 1:B:105:GLU:HG2 | 1:B:105:GLU:H   | 3        | 0.3           |
| (1,1281) | 1:B:105:GLU:HG3 | 1:B:105:GLU:H   | 3        | 0.3           |
| (1,1243) | 1:B:101:HIS:HB2 | 1:B:101:HIS:HD2 | 8        | 0.3           |
| (1,1204) | 1:B:98:ILE:HD11 | 1:B:98:ILE:HB   | 5        | 0.3           |
| (1,1204) | 1:B:98:ILE:HD12 | 1:B:98:ILE:HB   | 5        | 0.3           |
| (1,1204) | 1:B:98:ILE:HD13 | 1:B:98:ILE:HB   | 5        | 0.3           |
| (1,1198) | 1:B:97:VAL:HA   | 1:B:123:ARG:HD2 | 1        | 0.3           |
| (1,1198) | 1:B:97:VAL:HA   | 1:B:123:ARG:HD3 | 1        | 0.3           |
| (1,1181) | 1:B:96:ASP:HB2  | 1:B:96:ASP:H    | 2        | 0.3           |
| (1,1181) | 1:B:96:ASP:HB3  | 1:B:96:ASP:H    | 2        | 0.3           |
| (1,1180) | 1:B:96:ASP:HB2  | 1:B:96:ASP:H    | 2        | 0.3           |
| (1,1180) | 1:B:96:ASP:HB3  | 1:B:96:ASP:H    | 2        | 0.3           |
| (1,1178) | 1:B:96:ASP:HB2  | 1:B:96:ASP:H    | 2        | 0.3           |
| (1,1178) | 1:B:96:ASP:HB3  | 1:B:96:ASP:H    | 2        | 0.3           |
| (1,1173) | 1:B:95:GLY:HA2  | 1:B:97:VAL:H    | 7        | 0.3           |
| (1,1145) | 1:B:92:LYS:H    | 1:B:93:VAL:H    | 1        | 0.3           |
| (1,1145) | 1:B:92:LYS:H    | 1:B:93:VAL:H    | 3        | 0.3           |
| (1,1109) | 1:B:89:LEU:H    | 1:B:88:GLU:H    | 2        | 0.3           |
| (1,1108) | 1:B:89:LEU:H    | 1:B:88:GLU:H    | 2        | 0.3           |
| (1,1093) | 1:B:87:GLU:HG2  | 1:B:88:GLU:H    | 2        | 0.3           |
| (1,1093) | 1:B:87:GLU:HG3  | 1:B:88:GLU:H    | 2        | 0.3           |
| (1,108)  | 1:A:77:VAL:HG11 | 1:A:79:LEU:H    | 5        | 0.3           |
| (1,108)  | 1:A:77:VAL:HG12 | 1:A:79:LEU:H    | 5        | 0.3           |
| (1,108)  | 1:A:77:VAL:HG13 | 1:A:79:LEU:H    | 5        | 0.3           |
| (1,1068) | 1:B:84:PHE:HD1  | 1:B:89:LEU:HA   | 1        | 0.3           |
| (1,1068) | 1:B:84:PHE:HD2  | 1:B:89:LEU:HA   | 1        | 0.3           |
| (1,1049) | 1:B:83:HIS:HA   | 1:B:84:PHE:H    | 4        | 0.3           |
| (1,1048) | 1:B:83:HIS:HB2  | 1:B:84:PHE:HB2  | 2        | 0.3           |
| (1,1048) | 1:B:83:HIS:HB2  | 1:B:84:PHE:HB3  | 2        | 0.3           |
| (1,1042) | 1:B:83:HIS:HA   | 1:B:83:HIS:HB3  | 2        | 0.3           |
| (1,1041) | 1:B:83:HIS:HA   | 1:B:83:HIS:HB3  | 2        | 0.3           |
| (1,1030) | 1:B:81:VAL:HG21 | 1:B:83:HIS:H    | 2        | 0.3           |
| (1,1030) | 1:B:81:VAL:HG22 | 1:B:83:HIS:H    | 2        | 0.3           |
| (1,1030) | 1:B:81:VAL:HG23 | 1:B:83:HIS:H    | 2        | 0.3           |
| (1,1005) | 1:B:79:LEU:HD11 | 1:B:79:LEU:HA   | 6        | 0.3           |
| (1,1005) | 1:B:79:LEU:HD12 | 1:B:79:LEU:HA   | 6        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1005) | 1:B:79:LEU:HD13  | 1:B:79:LEU:HA    | 6        | 0.3           |
| (1,1005) | 1:B:79:LEU:HD21  | 1:B:79:LEU:HA    | 6        | 0.3           |
| (1,1005) | 1:B:79:LEU:HD22  | 1:B:79:LEU:HA    | 6        | 0.3           |
| (1,1005) | 1:B:79:LEU:HD23  | 1:B:79:LEU:HA    | 6        | 0.3           |
| (1,1005) | 1:B:79:LEU:HD11  | 1:B:79:LEU:HA    | 8        | 0.3           |
| (1,1005) | 1:B:79:LEU:HD12  | 1:B:79:LEU:HA    | 8        | 0.3           |
| (1,1005) | 1:B:79:LEU:HD13  | 1:B:79:LEU:HA    | 8        | 0.3           |
| (1,1005) | 1:B:79:LEU:HD21  | 1:B:79:LEU:HA    | 8        | 0.3           |
| (1,1005) | 1:B:79:LEU:HD22  | 1:B:79:LEU:HA    | 8        | 0.3           |
| (1,1005) | 1:B:79:LEU:HD23  | 1:B:79:LEU:HA    | 8        | 0.3           |
| (1,940)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2  | 7        | 0.29          |
| (1,937)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2  | 7        | 0.29          |
| (1,934)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2  | 7        | 0.29          |
| (1,918)  | 1:B:75:PHE:HA    | 1:B:76:SER:H     | 3        | 0.29          |
| (1,918)  | 1:B:75:PHE:HA    | 1:B:76:SER:H     | 6        | 0.29          |
| (1,918)  | 1:B:75:PHE:HA    | 1:B:76:SER:H     | 7        | 0.29          |
| (1,905)  | 1:B:74:ARG:H     | 1:B:73:ASP:H     | 6        | 0.29          |
| (1,904)  | 1:B:74:ARG:H     | 1:B:73:ASP:H     | 6        | 0.29          |
| (1,9)    | 1:A:68:MET:HE1   | 1:A:68:MET:H     | 3        | 0.29          |
| (1,9)    | 1:A:68:MET:HE2   | 1:A:68:MET:H     | 3        | 0.29          |
| (1,9)    | 1:A:68:MET:HE3   | 1:A:68:MET:H     | 3        | 0.29          |
| (1,876)  | 1:B:68:MET:HE1   | 1:B:68:MET:H     | 3        | 0.29          |
| (1,876)  | 1:B:68:MET:HE2   | 1:B:68:MET:H     | 3        | 0.29          |
| (1,876)  | 1:B:68:MET:HE3   | 1:B:68:MET:H     | 3        | 0.29          |
| (1,827)  | 1:A:146:ASP:HB3  | 1:A:76:SER:HA    | 7        | 0.29          |
| (1,826)  | 1:A:146:ASP:HB3  | 1:A:76:SER:HA    | 7        | 0.29          |
| (1,817)  | 1:A:145:VAL:HB   | 1:A:145:VAL:H    | 1        | 0.29          |
| (1,805)  | 1:A:144:THR:HG21 | 1:A:145:VAL:H    | 9        | 0.29          |
| (1,805)  | 1:A:144:THR:HG22 | 1:A:145:VAL:H    | 9        | 0.29          |
| (1,805)  | 1:A:144:THR:HG23 | 1:A:145:VAL:H    | 9        | 0.29          |
| (1,779)  | 1:A:142:VAL:HA   | 1:A:142:VAL:HG11 | 1        | 0.29          |
| (1,779)  | 1:A:142:VAL:HA   | 1:A:142:VAL:HG12 | 1        | 0.29          |
| (1,779)  | 1:A:142:VAL:HA   | 1:A:142:VAL:HG13 | 1        | 0.29          |
| (1,779)  | 1:A:142:VAL:HA   | 1:A:142:VAL:HG21 | 1        | 0.29          |
| (1,779)  | 1:A:142:VAL:HA   | 1:A:142:VAL:HG22 | 1        | 0.29          |
| (1,779)  | 1:A:142:VAL:HA   | 1:A:142:VAL:HG23 | 1        | 0.29          |
| (1,771)  | 1:A:141:GLY:HA2  | 1:A:141:GLY:H    | 1        | 0.29          |
| (1,745)  | 1:A:136:SER:H    | 1:A:135:SER:H    | 3        | 0.29          |
| (1,738)  | 1:A:135:SER:HA   | 1:A:145:VAL:HG21 | 7        | 0.29          |
| (1,738)  | 1:A:135:SER:HA   | 1:A:145:VAL:HG22 | 7        | 0.29          |
| (1,738)  | 1:A:135:SER:HA   | 1:A:145:VAL:HG23 | 7        | 0.29          |
| (1,73)   | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2  | 7        | 0.29          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,719) | 1:A:133:ILE:HG21 | 1:A:133:ILE:HA   | 4        | 0.29          |
| (1,719) | 1:A:133:ILE:HG22 | 1:A:133:ILE:HA   | 4        | 0.29          |
| (1,719) | 1:A:133:ILE:HG23 | 1:A:133:ILE:HA   | 4        | 0.29          |
| (1,708) | 1:A:132:THR:H    | 1:A:133:ILE:H    | 3        | 0.29          |
| (1,706) | 1:A:132:THR:H    | 1:A:133:ILE:H    | 3        | 0.29          |
| (1,70)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2  | 7        | 0.29          |
| (1,682) | 1:A:129:ASP:H    | 1:A:128:VAL:HA   | 2        | 0.29          |
| (1,67)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2  | 7        | 0.29          |
| (1,650) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HB   | 2        | 0.29          |
| (1,650) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HB   | 7        | 0.29          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD11 | 7        | 0.29          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD12 | 7        | 0.29          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD13 | 7        | 0.29          |
| (1,576) | 1:A:119:HIS:HB3  | 1:A:119:HIS:HA   | 6        | 0.29          |
| (1,575) | 1:A:119:HIS:HB3  | 1:A:119:HIS:HA   | 6        | 0.29          |
| (1,572) | 1:A:119:HIS:HB2  | 1:A:119:HIS:HA   | 4        | 0.29          |
| (1,572) | 1:A:119:HIS:HB2  | 1:A:119:HIS:HA   | 9        | 0.29          |
| (1,546) | 1:A:117:GLU:HA   | 1:A:117:GLU:H    | 9        | 0.29          |
| (1,518) | 1:A:114:ILE:HG21 | 1:A:114:ILE:H    | 5        | 0.29          |
| (1,518) | 1:A:114:ILE:HG22 | 1:A:114:ILE:H    | 5        | 0.29          |
| (1,518) | 1:A:114:ILE:HG23 | 1:A:114:ILE:H    | 5        | 0.29          |
| (1,51)  | 1:A:75:PHE:HA    | 1:A:76:SER:H     | 3        | 0.29          |
| (1,51)  | 1:A:75:PHE:HA    | 1:A:76:SER:H     | 6        | 0.29          |
| (1,51)  | 1:A:75:PHE:HA    | 1:A:76:SER:H     | 7        | 0.29          |
| (1,487) | 1:A:113:PHE:H    | 1:A:112:GLY:H    | 4        | 0.29          |
| (1,473) | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG21 | 7        | 0.29          |
| (1,473) | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG22 | 7        | 0.29          |
| (1,473) | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG23 | 7        | 0.29          |
| (1,465) | 1:A:111:HIS:HB2  | 1:A:111:HIS:H    | 7        | 0.29          |
| (1,454) | 1:A:110:GLU:H    | 1:A:110:GLU:HA   | 8        | 0.29          |
| (1,38)  | 1:A:74:ARG:H     | 1:A:73:ASP:H     | 6        | 0.29          |
| (1,378) | 1:A:101:HIS:HB3  | 1:A:101:HIS:H    | 8        | 0.29          |
| (1,37)  | 1:A:74:ARG:H     | 1:A:73:ASP:H     | 6        | 0.29          |
| (1,369) | 1:A:101:HIS:H    | 1:A:100:VAL:HA   | 3        | 0.29          |
| (1,335) | 1:A:98:ILE:H     | 1:A:97:VAL:H     | 6        | 0.29          |
| (1,314) | 1:A:96:ASP:HB2   | 1:A:96:ASP:H     | 9        | 0.29          |
| (1,314) | 1:A:96:ASP:HB3   | 1:A:96:ASP:H     | 9        | 0.29          |
| (1,313) | 1:A:96:ASP:HB2   | 1:A:96:ASP:H     | 9        | 0.29          |
| (1,313) | 1:A:96:ASP:HB3   | 1:A:96:ASP:H     | 9        | 0.29          |
| (1,311) | 1:A:96:ASP:HB2   | 1:A:96:ASP:H     | 9        | 0.29          |
| (1,311) | 1:A:96:ASP:HB3   | 1:A:96:ASP:H     | 9        | 0.29          |
| (1,279) | 1:A:92:LYS:H     | 1:A:99:GLU:H     | 5        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,278)  | 1:A:92:LYS:H     | 1:A:93:VAL:H     | 2        | 0.29          |
| (1,259)  | 1:A:89:LEU:HD11  | 1:A:103:LYS:H    | 7        | 0.29          |
| (1,259)  | 1:A:89:LEU:HD12  | 1:A:103:LYS:H    | 7        | 0.29          |
| (1,259)  | 1:A:89:LEU:HD13  | 1:A:103:LYS:H    | 7        | 0.29          |
| (1,175)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB3   | 8        | 0.29          |
| (1,174)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB3   | 8        | 0.29          |
| (1,1694) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA    | 7        | 0.29          |
| (1,1693) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA    | 7        | 0.29          |
| (1,1684) | 1:B:145:VAL:HB   | 1:B:145:VAL:H    | 1        | 0.29          |
| (1,1672) | 1:B:144:THR:HG21 | 1:B:145:VAL:H    | 9        | 0.29          |
| (1,1672) | 1:B:144:THR:HG22 | 1:B:145:VAL:H    | 9        | 0.29          |
| (1,1672) | 1:B:144:THR:HG23 | 1:B:145:VAL:H    | 9        | 0.29          |
| (1,1671) | 1:B:144:THR:HA   | 1:B:145:VAL:H    | 2        | 0.29          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG11 | 1        | 0.29          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG12 | 1        | 0.29          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG13 | 1        | 0.29          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG21 | 1        | 0.29          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG22 | 1        | 0.29          |
| (1,1646) | 1:B:142:VAL:HA   | 1:B:142:VAL:HG23 | 1        | 0.29          |
| (1,1638) | 1:B:141:GLY:HA2  | 1:B:141:GLY:H    | 1        | 0.29          |
| (1,1612) | 1:B:136:SER:H    | 1:B:135:SER:H    | 3        | 0.29          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG21 | 7        | 0.29          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG22 | 7        | 0.29          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG23 | 7        | 0.29          |
| (1,1586) | 1:B:133:ILE:HG21 | 1:B:133:ILE:HA   | 4        | 0.29          |
| (1,1586) | 1:B:133:ILE:HG22 | 1:B:133:ILE:HA   | 4        | 0.29          |
| (1,1586) | 1:B:133:ILE:HG23 | 1:B:133:ILE:HA   | 4        | 0.29          |
| (1,1575) | 1:B:132:THR:H    | 1:B:133:ILE:H    | 3        | 0.29          |
| (1,1573) | 1:B:132:THR:H    | 1:B:133:ILE:H    | 3        | 0.29          |
| (1,1549) | 1:B:129:ASP:H    | 1:B:128:VAL:HA   | 2        | 0.29          |
| (1,1517) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HB   | 7        | 0.29          |
| (1,1443) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA   | 6        | 0.29          |
| (1,1442) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA   | 6        | 0.29          |
| (1,1439) | 1:B:119:HIS:HB2  | 1:B:119:HIS:HA   | 4        | 0.29          |
| (1,1413) | 1:B:117:GLU:HA   | 1:B:117:GLU:H    | 9        | 0.29          |
| (1,1354) | 1:B:113:PHE:H    | 1:B:112:GLY:H    | 4        | 0.29          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG21 | 7        | 0.29          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG22 | 7        | 0.29          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG23 | 7        | 0.29          |
| (1,1332) | 1:B:111:HIS:HB2  | 1:B:111:HIS:H    | 7        | 0.29          |
| (1,1321) | 1:B:110:GLU:H    | 1:B:110:GLU:HA   | 8        | 0.29          |
| (1,1245) | 1:B:101:HIS:HB3  | 1:B:101:HIS:H    | 8        | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1236) | 1:B:101:HIS:H   | 1:B:100:VAL:HA  | 3        | 0.29          |
| (1,1218) | 1:B:99:GLU:HA   | 1:B:99:GLU:H    | 5        | 0.29          |
| (1,1202) | 1:B:98:ILE:H    | 1:B:97:VAL:H    | 6        | 0.29          |
| (1,1181) | 1:B:96:ASP:HB2  | 1:B:96:ASP:H    | 9        | 0.29          |
| (1,1181) | 1:B:96:ASP:HB3  | 1:B:96:ASP:H    | 9        | 0.29          |
| (1,1180) | 1:B:96:ASP:HB2  | 1:B:96:ASP:H    | 9        | 0.29          |
| (1,1180) | 1:B:96:ASP:HB3  | 1:B:96:ASP:H    | 9        | 0.29          |
| (1,1178) | 1:B:96:ASP:HB2  | 1:B:96:ASP:H    | 9        | 0.29          |
| (1,1178) | 1:B:96:ASP:HB3  | 1:B:96:ASP:H    | 9        | 0.29          |
| (1,1146) | 1:B:92:LYS:H    | 1:B:99:GLU:H    | 5        | 0.29          |
| (1,1145) | 1:B:92:LYS:H    | 1:B:93:VAL:H    | 2        | 0.29          |
| (1,1126) | 1:B:89:LEU:HD11 | 1:B:103:LYS:H   | 7        | 0.29          |
| (1,1126) | 1:B:89:LEU:HD12 | 1:B:103:LYS:H   | 7        | 0.29          |
| (1,1126) | 1:B:89:LEU:HD13 | 1:B:103:LYS:H   | 7        | 0.29          |
| (1,1042) | 1:B:83:HIS:HA   | 1:B:83:HIS:HB3  | 8        | 0.29          |
| (1,1041) | 1:B:83:HIS:HA   | 1:B:83:HIS:HB3  | 8        | 0.29          |
| (1,947)  | 1:B:77:VAL:HA   | 1:B:68:MET:HA   | 4        | 0.28          |
| (1,940)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2 | 3        | 0.28          |
| (1,937)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2 | 3        | 0.28          |
| (1,934)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2 | 3        | 0.28          |
| (1,921)  | 1:B:75:PHE:HD1  | 1:B:146:ASP:HB3 | 9        | 0.28          |
| (1,921)  | 1:B:75:PHE:HD2  | 1:B:146:ASP:HB3 | 9        | 0.28          |
| (1,905)  | 1:B:74:ARG:H    | 1:B:73:ASP:H    | 3        | 0.28          |
| (1,904)  | 1:B:74:ARG:H    | 1:B:73:ASP:H    | 3        | 0.28          |
| (1,898)  | 1:B:73:ASP:H    | 1:B:72:LYS:HB2  | 4        | 0.28          |
| (1,898)  | 1:B:73:ASP:H    | 1:B:72:LYS:HB3  | 4        | 0.28          |
| (1,895)  | 1:B:72:LYS:H    | 1:B:72:LYS:HA   | 2        | 0.28          |
| (1,872)  | 1:B:67:GLU:H    | 1:B:67:GLU:HA   | 1        | 0.28          |
| (1,872)  | 1:B:67:GLU:H    | 1:B:67:GLU:HA   | 6        | 0.28          |
| (1,80)   | 1:A:77:VAL:HA   | 1:A:68:MET:HA   | 4        | 0.28          |
| (1,771)  | 1:A:141:GLY:HA2 | 1:A:141:GLY:H   | 3        | 0.28          |
| (1,771)  | 1:A:141:GLY:HA2 | 1:A:141:GLY:H   | 8        | 0.28          |
| (1,752)  | 1:A:137:LEU:H   | 1:A:137:LEU:HB2 | 7        | 0.28          |
| (1,752)  | 1:A:137:LEU:H   | 1:A:137:LEU:HB3 | 7        | 0.28          |
| (1,73)   | 1:A:76:SER:HB2  | 1:A:146:ASP:HB2 | 3        | 0.28          |
| (1,708)  | 1:A:132:THR:H   | 1:A:133:ILE:H   | 2        | 0.28          |
| (1,706)  | 1:A:132:THR:H   | 1:A:133:ILE:H   | 2        | 0.28          |
| (1,70)   | 1:A:76:SER:HB2  | 1:A:146:ASP:HB2 | 3        | 0.28          |
| (1,695)  | 1:A:131:LEU:H   | 1:A:132:THR:H   | 2        | 0.28          |
| (1,694)  | 1:A:131:LEU:H   | 1:A:132:THR:H   | 2        | 0.28          |
| (1,67)   | 1:A:76:SER:HB2  | 1:A:146:ASP:HB2 | 3        | 0.28          |
| (1,572)  | 1:A:119:HIS:HB2 | 1:A:119:HIS:HA  | 7        | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,54)   | 1:A:75:PHE:HD1  | 1:A:146:ASP:HB3 | 9        | 0.28          |
| (1,54)   | 1:A:75:PHE:HD2  | 1:A:146:ASP:HB3 | 9        | 0.28          |
| (1,5)    | 1:A:67:GLU:H    | 1:A:67:GLU:HA   | 1        | 0.28          |
| (1,5)    | 1:A:67:GLU:H    | 1:A:67:GLU:HA   | 6        | 0.28          |
| (1,491)  | 1:A:113:PHE:HA  | 1:A:113:PHE:HB3 | 7        | 0.28          |
| (1,489)  | 1:A:113:PHE:HA  | 1:A:113:PHE:HB3 | 7        | 0.28          |
| (1,469)  | 1:A:111:HIS:HB2 | 1:A:112:GLY:H   | 8        | 0.28          |
| (1,469)  | 1:A:111:HIS:HB2 | 1:A:112:GLY:H   | 9        | 0.28          |
| (1,454)  | 1:A:110:GLU:H   | 1:A:110:GLU:HA  | 4        | 0.28          |
| (1,419)  | 1:A:105:GLU:HA  | 1:A:116:ARG:H   | 3        | 0.28          |
| (1,418)  | 1:A:105:GLU:HG2 | 1:A:115:SER:HB3 | 2        | 0.28          |
| (1,418)  | 1:A:105:GLU:HG3 | 1:A:115:SER:HB3 | 2        | 0.28          |
| (1,414)  | 1:A:105:GLU:HG2 | 1:A:105:GLU:H   | 4        | 0.28          |
| (1,414)  | 1:A:105:GLU:HG3 | 1:A:105:GLU:H   | 4        | 0.28          |
| (1,413)  | 1:A:105:GLU:HG2 | 1:A:105:GLU:H   | 4        | 0.28          |
| (1,413)  | 1:A:105:GLU:HG3 | 1:A:105:GLU:H   | 4        | 0.28          |
| (1,399)  | 1:A:103:LYS:HA  | 1:A:118:PHE:H   | 5        | 0.28          |
| (1,390)  | 1:A:102:GLY:HA2 | 1:A:103:LYS:H   | 3        | 0.28          |
| (1,38)   | 1:A:74:ARG:H    | 1:A:73:ASP:H    | 3        | 0.28          |
| (1,37)   | 1:A:74:ARG:H    | 1:A:73:ASP:H    | 3        | 0.28          |
| (1,351)  | 1:A:99:GLU:HA   | 1:A:99:GLU:H    | 4        | 0.28          |
| (1,351)  | 1:A:99:GLU:HA   | 1:A:99:GLU:H    | 5        | 0.28          |
| (1,31)   | 1:A:73:ASP:H    | 1:A:72:LYS:HB2  | 4        | 0.28          |
| (1,31)   | 1:A:73:ASP:H    | 1:A:72:LYS:HB3  | 4        | 0.28          |
| (1,306)  | 1:A:95:GLY:HA2  | 1:A:97:VAL:H    | 9        | 0.28          |
| (1,281)  | 1:A:92:LYS:H    | 1:A:101:HIS:H   | 6        | 0.28          |
| (1,28)   | 1:A:72:LYS:H    | 1:A:72:LYS:HA   | 2        | 0.28          |
| (1,267)  | 1:A:90:LYS:HB2  | 1:A:101:HIS:HB3 | 1        | 0.28          |
| (1,267)  | 1:A:90:LYS:HB3  | 1:A:101:HIS:HB3 | 1        | 0.28          |
| (1,228)  | 1:A:87:GLU:H    | 1:A:88:GLU:H    | 4        | 0.28          |
| (1,226)  | 1:A:87:GLU:HG2  | 1:A:88:GLU:H    | 5        | 0.28          |
| (1,226)  | 1:A:87:GLU:HG3  | 1:A:88:GLU:H    | 5        | 0.28          |
| (1,225)  | 1:A:87:GLU:H    | 1:A:88:GLU:H    | 4        | 0.28          |
| (1,191)  | 1:A:84:PHE:HD1  | 1:A:82:LYS:H    | 8        | 0.28          |
| (1,191)  | 1:A:84:PHE:HD2  | 1:A:82:LYS:H    | 8        | 0.28          |
| (1,164)  | 1:A:81:VAL:HG21 | 1:A:84:PHE:H    | 1        | 0.28          |
| (1,164)  | 1:A:81:VAL:HG22 | 1:A:84:PHE:H    | 1        | 0.28          |
| (1,164)  | 1:A:81:VAL:HG23 | 1:A:84:PHE:H    | 1        | 0.28          |
| (1,1638) | 1:B:141:GLY:HA2 | 1:B:141:GLY:H   | 3        | 0.28          |
| (1,1638) | 1:B:141:GLY:HA2 | 1:B:141:GLY:H   | 8        | 0.28          |
| (1,1619) | 1:B:137:LEU:H   | 1:B:137:LEU:HB2 | 7        | 0.28          |
| (1,1619) | 1:B:137:LEU:H   | 1:B:137:LEU:HB3 | 7        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG21 | 4        | 0.28          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG22 | 4        | 0.28          |
| (1,1605) | 1:B:135:SER:HA   | 1:B:145:VAL:HG23 | 4        | 0.28          |
| (1,1586) | 1:B:133:ILE:HG21 | 1:B:133:ILE:HA   | 3        | 0.28          |
| (1,1586) | 1:B:133:ILE:HG22 | 1:B:133:ILE:HA   | 3        | 0.28          |
| (1,1586) | 1:B:133:ILE:HG23 | 1:B:133:ILE:HA   | 3        | 0.28          |
| (1,1586) | 1:B:133:ILE:HG21 | 1:B:133:ILE:HA   | 8        | 0.28          |
| (1,1586) | 1:B:133:ILE:HG22 | 1:B:133:ILE:HA   | 8        | 0.28          |
| (1,1586) | 1:B:133:ILE:HG23 | 1:B:133:ILE:HA   | 8        | 0.28          |
| (1,1575) | 1:B:132:THR:H    | 1:B:133:ILE:H    | 2        | 0.28          |
| (1,1573) | 1:B:132:THR:H    | 1:B:133:ILE:H    | 2        | 0.28          |
| (1,1562) | 1:B:131:LEU:H    | 1:B:132:THR:H    | 2        | 0.28          |
| (1,1561) | 1:B:131:LEU:H    | 1:B:132:THR:H    | 2        | 0.28          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD11 | 7        | 0.28          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD12 | 7        | 0.28          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD13 | 7        | 0.28          |
| (1,1439) | 1:B:119:HIS:HB2  | 1:B:119:HIS:HA   | 7        | 0.28          |
| (1,1439) | 1:B:119:HIS:HB2  | 1:B:119:HIS:HA   | 9        | 0.28          |
| (1,1358) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3  | 7        | 0.28          |
| (1,1356) | 1:B:113:PHE:HA   | 1:B:113:PHE:HB3  | 7        | 0.28          |
| (1,1336) | 1:B:111:HIS:HB2  | 1:B:112:GLY:H    | 8        | 0.28          |
| (1,1336) | 1:B:111:HIS:HB2  | 1:B:112:GLY:H    | 9        | 0.28          |
| (1,1321) | 1:B:110:GLU:H    | 1:B:110:GLU:HA   | 4        | 0.28          |
| (1,1286) | 1:B:105:GLU:HA   | 1:B:116:ARG:H    | 3        | 0.28          |
| (1,1285) | 1:B:105:GLU:HG2  | 1:B:115:SER:HB3  | 2        | 0.28          |
| (1,1285) | 1:B:105:GLU:HG3  | 1:B:115:SER:HB3  | 2        | 0.28          |
| (1,1281) | 1:B:105:GLU:HG2  | 1:B:105:GLU:H    | 4        | 0.28          |
| (1,1281) | 1:B:105:GLU:HG3  | 1:B:105:GLU:H    | 4        | 0.28          |
| (1,1280) | 1:B:105:GLU:HG2  | 1:B:105:GLU:H    | 4        | 0.28          |
| (1,1280) | 1:B:105:GLU:HG3  | 1:B:105:GLU:H    | 4        | 0.28          |
| (1,1266) | 1:B:103:LYS:HA   | 1:B:118:PHE:H    | 5        | 0.28          |
| (1,1257) | 1:B:102:GLY:HA2  | 1:B:103:LYS:H    | 3        | 0.28          |
| (1,1218) | 1:B:99:GLU:HA    | 1:B:99:GLU:H     | 4        | 0.28          |
| (1,1173) | 1:B:95:GLY:HA2   | 1:B:97:VAL:H     | 9        | 0.28          |
| (1,1148) | 1:B:92:LYS:H     | 1:B:101:HIS:H    | 6        | 0.28          |
| (1,1095) | 1:B:87:GLU:H     | 1:B:88:GLU:H     | 4        | 0.28          |
| (1,1093) | 1:B:87:GLU:HG2   | 1:B:88:GLU:H     | 5        | 0.28          |
| (1,1093) | 1:B:87:GLU:HG3   | 1:B:88:GLU:H     | 5        | 0.28          |
| (1,1092) | 1:B:87:GLU:H     | 1:B:88:GLU:H     | 4        | 0.28          |
| (1,1058) | 1:B:84:PHE:HD1   | 1:B:82:LYS:H     | 8        | 0.28          |
| (1,1058) | 1:B:84:PHE:HD2   | 1:B:82:LYS:H     | 8        | 0.28          |
| (1,1031) | 1:B:81:VAL:HG21  | 1:B:84:PHE:H     | 1        | 0.28          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1031) | 1:B:81:VAL:HG22 | 1:B:84:PHE:H     | 1        | 0.28          |
| (1,1031) | 1:B:81:VAL:HG23 | 1:B:84:PHE:H     | 1        | 0.28          |
| (1,981)  | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG11 | 8        | 0.27          |
| (1,981)  | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG12 | 8        | 0.27          |
| (1,981)  | 1:B:77:VAL:HG21 | 1:B:145:VAL:HG13 | 8        | 0.27          |
| (1,981)  | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG11 | 8        | 0.27          |
| (1,981)  | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG12 | 8        | 0.27          |
| (1,981)  | 1:B:77:VAL:HG22 | 1:B:145:VAL:HG13 | 8        | 0.27          |
| (1,981)  | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG11 | 8        | 0.27          |
| (1,981)  | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG12 | 8        | 0.27          |
| (1,981)  | 1:B:77:VAL:HG23 | 1:B:145:VAL:HG13 | 8        | 0.27          |
| (1,972)  | 1:B:77:VAL:HG21 | 1:B:79:LEU:HG    | 2        | 0.27          |
| (1,972)  | 1:B:77:VAL:HG22 | 1:B:79:LEU:HG    | 2        | 0.27          |
| (1,972)  | 1:B:77:VAL:HG23 | 1:B:79:LEU:HG    | 2        | 0.27          |
| (1,970)  | 1:B:77:VAL:H    | 1:B:78:ASN:H     | 2        | 0.27          |
| (1,97)   | 1:A:77:VAL:HG21 | 1:A:77:VAL:H     | 5        | 0.27          |
| (1,97)   | 1:A:77:VAL:HG22 | 1:A:77:VAL:H     | 5        | 0.27          |
| (1,97)   | 1:A:77:VAL:HG23 | 1:A:77:VAL:H     | 5        | 0.27          |
| (1,964)  | 1:B:77:VAL:HG21 | 1:B:77:VAL:H     | 5        | 0.27          |
| (1,964)  | 1:B:77:VAL:HG22 | 1:B:77:VAL:H     | 5        | 0.27          |
| (1,964)  | 1:B:77:VAL:HG23 | 1:B:77:VAL:H     | 5        | 0.27          |
| (1,947)  | 1:B:77:VAL:HA   | 1:B:68:MET:HA    | 7        | 0.27          |
| (1,913)  | 1:B:75:PHE:HA   | 1:B:75:PHE:HB2   | 2        | 0.27          |
| (1,872)  | 1:B:67:GLU:H    | 1:B:67:GLU:HA    | 9        | 0.27          |
| (1,829)  | 1:A:146:ASP:H   | 1:A:134:THR:H    | 2        | 0.27          |
| (1,828)  | 1:A:146:ASP:H   | 1:A:134:THR:H    | 2        | 0.27          |
| (1,827)  | 1:A:146:ASP:HB3 | 1:A:76:SER:HA    | 5        | 0.27          |
| (1,826)  | 1:A:146:ASP:HB3 | 1:A:76:SER:HA    | 5        | 0.27          |
| (1,825)  | 1:A:146:ASP:HB2 | 1:A:76:SER:HA    | 6        | 0.27          |
| (1,824)  | 1:A:146:ASP:HB2 | 1:A:76:SER:HA    | 6        | 0.27          |
| (1,812)  | 1:A:145:VAL:HB  | 1:A:135:SER:HA   | 9        | 0.27          |
| (1,80)   | 1:A:77:VAL:HA   | 1:A:68:MET:HA    | 7        | 0.27          |
| (1,771)  | 1:A:141:GLY:HA2 | 1:A:141:GLY:H    | 2        | 0.27          |
| (1,752)  | 1:A:137:LEU:H   | 1:A:137:LEU:HB2  | 5        | 0.27          |
| (1,752)  | 1:A:137:LEU:H   | 1:A:137:LEU:HB3  | 5        | 0.27          |
| (1,749)  | 1:A:136:SER:HA  | 1:A:137:LEU:H    | 1        | 0.27          |
| (1,749)  | 1:A:136:SER:HA  | 1:A:137:LEU:H    | 4        | 0.27          |
| (1,749)  | 1:A:136:SER:HA  | 1:A:137:LEU:H    | 8        | 0.27          |
| (1,745)  | 1:A:136:SER:H   | 1:A:135:SER:H    | 5        | 0.27          |
| (1,745)  | 1:A:136:SER:H   | 1:A:135:SER:H    | 6        | 0.27          |
| (1,729)  | 1:A:134:THR:H   | 1:A:134:THR:HG21 | 7        | 0.27          |
| (1,729)  | 1:A:134:THR:H   | 1:A:134:THR:HG22 | 7        | 0.27          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,729) | 1:A:134:THR:H    | 1:A:134:THR:HG23 | 7        | 0.27          |
| (1,728) | 1:A:133:ILE:HG12 | 1:A:147:GLY:HA2  | 8        | 0.27          |
| (1,728) | 1:A:133:ILE:HG13 | 1:A:147:GLY:HA2  | 8        | 0.27          |
| (1,719) | 1:A:133:ILE:HG21 | 1:A:133:ILE:HA   | 3        | 0.27          |
| (1,719) | 1:A:133:ILE:HG22 | 1:A:133:ILE:HA   | 3        | 0.27          |
| (1,719) | 1:A:133:ILE:HG23 | 1:A:133:ILE:HA   | 3        | 0.27          |
| (1,719) | 1:A:133:ILE:HG21 | 1:A:133:ILE:HA   | 8        | 0.27          |
| (1,719) | 1:A:133:ILE:HG22 | 1:A:133:ILE:HA   | 8        | 0.27          |
| (1,719) | 1:A:133:ILE:HG23 | 1:A:133:ILE:HA   | 8        | 0.27          |
| (1,708) | 1:A:132:THR:H    | 1:A:133:ILE:H    | 9        | 0.27          |
| (1,706) | 1:A:132:THR:H    | 1:A:133:ILE:H    | 9        | 0.27          |
| (1,682) | 1:A:129:ASP:H    | 1:A:128:VAL:HA   | 8        | 0.27          |
| (1,573) | 1:A:119:HIS:HA   | 1:A:119:HIS:HD2  | 9        | 0.27          |
| (1,546) | 1:A:117:GLU:HA   | 1:A:117:GLU:H    | 6        | 0.27          |
| (1,546) | 1:A:117:GLU:HA   | 1:A:117:GLU:H    | 8        | 0.27          |
| (1,513) | 1:A:114:ILE:HA   | 1:A:114:ILE:HB   | 4        | 0.27          |
| (1,501) | 1:A:114:ILE:HD11 | 1:A:104:HIS:HE1  | 3        | 0.27          |
| (1,501) | 1:A:114:ILE:HD12 | 1:A:104:HIS:HE1  | 3        | 0.27          |
| (1,501) | 1:A:114:ILE:HD13 | 1:A:104:HIS:HE1  | 3        | 0.27          |
| (1,5)   | 1:A:67:GLU:H     | 1:A:67:GLU:HA    | 9        | 0.27          |
| (1,494) | 1:A:113:PHE:HA   | 1:A:113:PHE:HD1  | 1        | 0.27          |
| (1,494) | 1:A:113:PHE:HA   | 1:A:113:PHE:HD2  | 1        | 0.27          |
| (1,487) | 1:A:113:PHE:H    | 1:A:112:GLY:H    | 7        | 0.27          |
| (1,482) | 1:A:113:PHE:HD1  | 1:A:107:ARG:HA   | 8        | 0.27          |
| (1,482) | 1:A:113:PHE:HD2  | 1:A:107:ARG:HA   | 8        | 0.27          |
| (1,447) | 1:A:109:ASP:H    | 1:A:109:ASP:HB2  | 5        | 0.27          |
| (1,447) | 1:A:109:ASP:H    | 1:A:109:ASP:HB3  | 5        | 0.27          |
| (1,378) | 1:A:101:HIS:HB3  | 1:A:101:HIS:H    | 4        | 0.27          |
| (1,360) | 1:A:100:VAL:HA   | 1:A:100:VAL:H    | 5        | 0.27          |
| (1,351) | 1:A:99:GLU:HA    | 1:A:99:GLU:H     | 7        | 0.27          |
| (1,339) | 1:A:98:ILE:HB    | 1:A:98:ILE:H     | 2        | 0.27          |
| (1,332) | 1:A:97:VAL:HA    | 1:A:124:ILE:HG12 | 3        | 0.27          |
| (1,332) | 1:A:97:VAL:HA    | 1:A:124:ILE:HG13 | 3        | 0.27          |
| (1,292) | 1:A:94:LEU:HD11  | 1:A:95:GLY:H     | 3        | 0.27          |
| (1,292) | 1:A:94:LEU:HD12  | 1:A:95:GLY:H     | 3        | 0.27          |
| (1,292) | 1:A:94:LEU:HD13  | 1:A:95:GLY:H     | 3        | 0.27          |
| (1,292) | 1:A:94:LEU:HD21  | 1:A:95:GLY:H     | 3        | 0.27          |
| (1,292) | 1:A:94:LEU:HD22  | 1:A:95:GLY:H     | 3        | 0.27          |
| (1,292) | 1:A:94:LEU:HD23  | 1:A:95:GLY:H     | 3        | 0.27          |
| (1,280) | 1:A:92:LYS:H     | 1:A:100:VAL:HA   | 6        | 0.27          |
| (1,275) | 1:A:92:LYS:H     | 1:A:92:LYS:HG2   | 4        | 0.27          |
| (1,275) | 1:A:92:LYS:H     | 1:A:92:LYS:HG3   | 4        | 0.27          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,267)  | 1:A:90:LYS:HB2   | 1:A:101:HIS:HB3 | 8        | 0.27          |
| (1,267)  | 1:A:90:LYS:HB3   | 1:A:101:HIS:HB3 | 8        | 0.27          |
| (1,252)  | 1:A:89:LEU:H     | 1:A:90:LYS:H    | 9        | 0.27          |
| (1,231)  | 1:A:87:GLU:HB2   | 1:A:89:LEU:H    | 2        | 0.27          |
| (1,231)  | 1:A:87:GLU:HB3   | 1:A:89:LEU:H    | 2        | 0.27          |
| (1,226)  | 1:A:87:GLU:HG2   | 1:A:88:GLU:H    | 9        | 0.27          |
| (1,226)  | 1:A:87:GLU:HG3   | 1:A:88:GLU:H    | 9        | 0.27          |
| (1,216)  | 1:A:85:SER:HB2   | 1:A:89:LEU:H    | 4        | 0.27          |
| (1,173)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HD2  | 9        | 0.27          |
| (1,1696) | 1:B:146:ASP:H    | 1:B:134:THR:H   | 2        | 0.27          |
| (1,1695) | 1:B:146:ASP:H    | 1:B:134:THR:H   | 2        | 0.27          |
| (1,1694) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA   | 5        | 0.27          |
| (1,1693) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA   | 5        | 0.27          |
| (1,1692) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA   | 6        | 0.27          |
| (1,1691) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA   | 6        | 0.27          |
| (1,1679) | 1:B:145:VAL:HB   | 1:B:135:SER:HA  | 9        | 0.27          |
| (1,1638) | 1:B:141:GLY:HA2  | 1:B:141:GLY:H   | 2        | 0.27          |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB2 | 5        | 0.27          |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB3 | 5        | 0.27          |
| (1,1616) | 1:B:136:SER:HA   | 1:B:137:LEU:H   | 1        | 0.27          |
| (1,1616) | 1:B:136:SER:HA   | 1:B:137:LEU:H   | 4        | 0.27          |
| (1,1616) | 1:B:136:SER:HA   | 1:B:137:LEU:H   | 8        | 0.27          |
| (1,1612) | 1:B:136:SER:H    | 1:B:135:SER:H   | 5        | 0.27          |
| (1,1612) | 1:B:136:SER:H    | 1:B:135:SER:H   | 6        | 0.27          |
| (1,1595) | 1:B:133:ILE:HG12 | 1:B:147:GLY:HA2 | 8        | 0.27          |
| (1,1595) | 1:B:133:ILE:HG13 | 1:B:147:GLY:HA2 | 8        | 0.27          |
| (1,1575) | 1:B:132:THR:H    | 1:B:133:ILE:H   | 9        | 0.27          |
| (1,1573) | 1:B:132:THR:H    | 1:B:133:ILE:H   | 9        | 0.27          |
| (1,1549) | 1:B:129:ASP:H    | 1:B:128:VAL:HA  | 8        | 0.27          |
| (1,1413) | 1:B:117:GLU:HA   | 1:B:117:GLU:H   | 6        | 0.27          |
| (1,1413) | 1:B:117:GLU:HA   | 1:B:117:GLU:H   | 8        | 0.27          |
| (1,1380) | 1:B:114:ILE:HA   | 1:B:114:ILE:HB  | 4        | 0.27          |
| (1,138)  | 1:A:79:LEU:HD11  | 1:A:79:LEU:HA   | 2        | 0.27          |
| (1,138)  | 1:A:79:LEU:HD12  | 1:A:79:LEU:HA   | 2        | 0.27          |
| (1,138)  | 1:A:79:LEU:HD13  | 1:A:79:LEU:HA   | 2        | 0.27          |
| (1,138)  | 1:A:79:LEU:HD21  | 1:A:79:LEU:HA   | 2        | 0.27          |
| (1,138)  | 1:A:79:LEU:HD22  | 1:A:79:LEU:HA   | 2        | 0.27          |
| (1,138)  | 1:A:79:LEU:HD23  | 1:A:79:LEU:HA   | 2        | 0.27          |
| (1,1368) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HE1 | 3        | 0.27          |
| (1,1368) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HE1 | 3        | 0.27          |
| (1,1368) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HE1 | 3        | 0.27          |
| (1,1361) | 1:B:113:PHE:HA   | 1:B:113:PHE:HD1 | 1        | 0.27          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1361) | 1:B:113:PHE:HA  | 1:B:113:PHE:HD2  | 1        | 0.27          |
| (1,1354) | 1:B:113:PHE:H   | 1:B:112:GLY:H    | 7        | 0.27          |
| (1,1349) | 1:B:113:PHE:HD1 | 1:B:107:ARG:HA   | 8        | 0.27          |
| (1,1349) | 1:B:113:PHE:HD2 | 1:B:107:ARG:HA   | 8        | 0.27          |
| (1,1245) | 1:B:101:HIS:HB3 | 1:B:101:HIS:H    | 4        | 0.27          |
| (1,1218) | 1:B:99:GLU:HA   | 1:B:99:GLU:H     | 7        | 0.27          |
| (1,1206) | 1:B:98:ILE:HB   | 1:B:98:ILE:H     | 2        | 0.27          |
| (1,1199) | 1:B:97:VAL:HA   | 1:B:124:ILE:HG12 | 3        | 0.27          |
| (1,1199) | 1:B:97:VAL:HA   | 1:B:124:ILE:HG13 | 3        | 0.27          |
| (1,1159) | 1:B:94:LEU:HD11 | 1:B:95:GLY:H     | 3        | 0.27          |
| (1,1159) | 1:B:94:LEU:HD12 | 1:B:95:GLY:H     | 3        | 0.27          |
| (1,1159) | 1:B:94:LEU:HD13 | 1:B:95:GLY:H     | 3        | 0.27          |
| (1,1159) | 1:B:94:LEU:HD21 | 1:B:95:GLY:H     | 3        | 0.27          |
| (1,1159) | 1:B:94:LEU:HD22 | 1:B:95:GLY:H     | 3        | 0.27          |
| (1,1159) | 1:B:94:LEU:HD23 | 1:B:95:GLY:H     | 3        | 0.27          |
| (1,1147) | 1:B:92:LYS:H    | 1:B:100:VAL:HA   | 6        | 0.27          |
| (1,1142) | 1:B:92:LYS:H    | 1:B:92:LYS:HG2   | 4        | 0.27          |
| (1,1142) | 1:B:92:LYS:H    | 1:B:92:LYS:HG3   | 4        | 0.27          |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG11 | 8        | 0.27          |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG12 | 8        | 0.27          |
| (1,114)  | 1:A:77:VAL:HG21 | 1:A:145:VAL:HG13 | 8        | 0.27          |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG11 | 8        | 0.27          |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG12 | 8        | 0.27          |
| (1,114)  | 1:A:77:VAL:HG22 | 1:A:145:VAL:HG13 | 8        | 0.27          |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG11 | 8        | 0.27          |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG12 | 8        | 0.27          |
| (1,114)  | 1:A:77:VAL:HG23 | 1:A:145:VAL:HG13 | 8        | 0.27          |
| (1,1134) | 1:B:90:LYS:HB2  | 1:B:101:HIS:HB3  | 1        | 0.27          |
| (1,1134) | 1:B:90:LYS:HB3  | 1:B:101:HIS:HB3  | 1        | 0.27          |
| (1,1134) | 1:B:90:LYS:HB2  | 1:B:101:HIS:HB3  | 8        | 0.27          |
| (1,1134) | 1:B:90:LYS:HB3  | 1:B:101:HIS:HB3  | 8        | 0.27          |
| (1,1119) | 1:B:89:LEU:H    | 1:B:90:LYS:H     | 9        | 0.27          |
| (1,1098) | 1:B:87:GLU:HB2  | 1:B:89:LEU:H     | 2        | 0.27          |
| (1,1098) | 1:B:87:GLU:HB3  | 1:B:89:LEU:H     | 2        | 0.27          |
| (1,1093) | 1:B:87:GLU:HG2  | 1:B:88:GLU:H     | 9        | 0.27          |
| (1,1093) | 1:B:87:GLU:HG3  | 1:B:88:GLU:H     | 9        | 0.27          |
| (1,1083) | 1:B:85:SER:HB2  | 1:B:89:LEU:H     | 4        | 0.27          |
| (1,105)  | 1:A:77:VAL:HG21 | 1:A:79:LEU:HG    | 2        | 0.27          |
| (1,105)  | 1:A:77:VAL:HG22 | 1:A:79:LEU:HG    | 2        | 0.27          |
| (1,105)  | 1:A:77:VAL:HG23 | 1:A:79:LEU:HG    | 2        | 0.27          |
| (1,103)  | 1:A:77:VAL:H    | 1:A:78:ASN:H     | 2        | 0.27          |
| (1,1005) | 1:B:79:LEU:HD11 | 1:B:79:LEU:HA    | 2        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1005) | 1:B:79:LEU:HD12  | 1:B:79:LEU:HA    | 2        | 0.27          |
| (1,1005) | 1:B:79:LEU:HD13  | 1:B:79:LEU:HA    | 2        | 0.27          |
| (1,1005) | 1:B:79:LEU:HD21  | 1:B:79:LEU:HA    | 2        | 0.27          |
| (1,1005) | 1:B:79:LEU:HD22  | 1:B:79:LEU:HA    | 2        | 0.27          |
| (1,1005) | 1:B:79:LEU:HD23  | 1:B:79:LEU:HA    | 2        | 0.27          |
| (1,996)  | 1:B:78:ASN:HB3   | 1:B:79:LEU:H     | 4        | 0.26          |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD11  | 9        | 0.26          |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD12  | 9        | 0.26          |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD13  | 9        | 0.26          |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD21  | 9        | 0.26          |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD22  | 9        | 0.26          |
| (1,994)  | 1:B:78:ASN:HA    | 1:B:79:LEU:HD23  | 9        | 0.26          |
| (1,972)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HG    | 6        | 0.26          |
| (1,972)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HG    | 6        | 0.26          |
| (1,972)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HG    | 6        | 0.26          |
| (1,97)   | 1:A:77:VAL:HG21  | 1:A:77:VAL:H     | 1        | 0.26          |
| (1,97)   | 1:A:77:VAL:HG22  | 1:A:77:VAL:H     | 1        | 0.26          |
| (1,97)   | 1:A:77:VAL:HG23  | 1:A:77:VAL:H     | 1        | 0.26          |
| (1,940)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2  | 9        | 0.26          |
| (1,937)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2  | 9        | 0.26          |
| (1,934)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2  | 9        | 0.26          |
| (1,854)  | 1:A:148:PRO:HB2  | 1:A:149:ARG:H    | 7        | 0.26          |
| (1,854)  | 1:A:148:PRO:HB3  | 1:A:149:ARG:H    | 7        | 0.26          |
| (1,827)  | 1:A:146:ASP:HB3  | 1:A:76:SER:HA    | 4        | 0.26          |
| (1,826)  | 1:A:146:ASP:HB3  | 1:A:76:SER:HA    | 4        | 0.26          |
| (1,817)  | 1:A:145:VAL:HB   | 1:A:145:VAL:H    | 6        | 0.26          |
| (1,808)  | 1:A:144:THR:H    | 1:A:145:VAL:H    | 8        | 0.26          |
| (1,803)  | 1:A:144:THR:H    | 1:A:145:VAL:H    | 8        | 0.26          |
| (1,785)  | 1:A:142:VAL:HG11 | 1:A:143:LEU:H    | 6        | 0.26          |
| (1,785)  | 1:A:142:VAL:HG12 | 1:A:143:LEU:H    | 6        | 0.26          |
| (1,785)  | 1:A:142:VAL:HG13 | 1:A:143:LEU:H    | 6        | 0.26          |
| (1,785)  | 1:A:142:VAL:HG21 | 1:A:143:LEU:H    | 6        | 0.26          |
| (1,785)  | 1:A:142:VAL:HG22 | 1:A:143:LEU:H    | 6        | 0.26          |
| (1,785)  | 1:A:142:VAL:HG23 | 1:A:143:LEU:H    | 6        | 0.26          |
| (1,771)  | 1:A:141:GLY:HA2  | 1:A:141:GLY:H    | 6        | 0.26          |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB2  | 3        | 0.26          |
| (1,752)  | 1:A:137:LEU:H    | 1:A:137:LEU:HB3  | 3        | 0.26          |
| (1,73)   | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2  | 9        | 0.26          |
| (1,70)   | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2  | 9        | 0.26          |
| (1,67)   | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2  | 9        | 0.26          |
| (1,650)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HB   | 3        | 0.26          |
| (1,647)  | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD11 | 3        | 0.26          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,647)  | 1:A:125:PRO:HD3 | 1:A:124:ILE:HD12 | 3        | 0.26          |
| (1,647)  | 1:A:125:PRO:HD3 | 1:A:124:ILE:HD13 | 3        | 0.26          |
| (1,609)  | 1:A:123:ARG:HA  | 1:A:123:ARG:HD2  | 5        | 0.26          |
| (1,609)  | 1:A:123:ARG:HA  | 1:A:123:ARG:HD3  | 5        | 0.26          |
| (1,600)  | 1:A:122:TYR:HA  | 1:A:123:ARG:HB3  | 8        | 0.26          |
| (1,593)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:HA   | 2        | 0.26          |
| (1,593)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:HA   | 2        | 0.26          |
| (1,591)  | 1:A:122:TYR:HB2 | 1:A:122:TYR:HA   | 2        | 0.26          |
| (1,591)  | 1:A:122:TYR:HB3 | 1:A:122:TYR:HA   | 2        | 0.26          |
| (1,588)  | 1:A:122:TYR:HB2 | 1:A:98:ILE:HD11  | 9        | 0.26          |
| (1,588)  | 1:A:122:TYR:HB2 | 1:A:98:ILE:HD12  | 9        | 0.26          |
| (1,588)  | 1:A:122:TYR:HB2 | 1:A:98:ILE:HD13  | 9        | 0.26          |
| (1,588)  | 1:A:122:TYR:HB3 | 1:A:98:ILE:HD11  | 9        | 0.26          |
| (1,588)  | 1:A:122:TYR:HB3 | 1:A:98:ILE:HD12  | 9        | 0.26          |
| (1,588)  | 1:A:122:TYR:HB3 | 1:A:98:ILE:HD13  | 9        | 0.26          |
| (1,579)  | 1:A:119:HIS:H   | 1:A:120:ARG:H    | 5        | 0.26          |
| (1,576)  | 1:A:119:HIS:HB3 | 1:A:119:HIS:HA   | 2        | 0.26          |
| (1,575)  | 1:A:119:HIS:HB3 | 1:A:119:HIS:HA   | 2        | 0.26          |
| (1,550)  | 1:A:118:PHE:HE1 | 1:A:102:GLY:H    | 7        | 0.26          |
| (1,550)  | 1:A:118:PHE:HE2 | 1:A:102:GLY:H    | 7        | 0.26          |
| (1,546)  | 1:A:117:GLU:HA  | 1:A:117:GLU:H    | 7        | 0.26          |
| (1,487)  | 1:A:113:PHE:H   | 1:A:112:GLY:H    | 2        | 0.26          |
| (1,469)  | 1:A:111:HIS:HB2 | 1:A:112:GLY:H    | 2        | 0.26          |
| (1,46)   | 1:A:75:PHE:HA   | 1:A:75:PHE:HB2   | 2        | 0.26          |
| (1,405)  | 1:A:104:HIS:HB3 | 1:A:104:HIS:HA   | 3        | 0.26          |
| (1,404)  | 1:A:104:HIS:HB3 | 1:A:104:HIS:HA   | 3        | 0.26          |
| (1,390)  | 1:A:102:GLY:HA2 | 1:A:103:LYS:H    | 9        | 0.26          |
| (1,301)  | 1:A:95:GLY:H    | 1:A:94:LEU:HG    | 8        | 0.26          |
| (1,289)  | 1:A:94:LEU:H    | 1:A:93:VAL:HB    | 2        | 0.26          |
| (1,289)  | 1:A:94:LEU:H    | 1:A:93:VAL:HB    | 6        | 0.26          |
| (1,289)  | 1:A:94:LEU:H    | 1:A:93:VAL:HB    | 9        | 0.26          |
| (1,281)  | 1:A:92:LYS:H    | 1:A:101:HIS:H    | 3        | 0.26          |
| (1,278)  | 1:A:92:LYS:H    | 1:A:93:VAL:H     | 6        | 0.26          |
| (1,272)  | 1:A:92:LYS:H    | 1:A:91:VAL:HA    | 7        | 0.26          |
| (1,253)  | 1:A:89:LEU:HA   | 1:A:90:LYS:H     | 1        | 0.26          |
| (1,218)  | 1:A:86:PRO:HB2  | 1:A:85:SER:HA    | 4        | 0.26          |
| (1,218)  | 1:A:86:PRO:HB3  | 1:A:85:SER:HA    | 4        | 0.26          |
| (1,1760) | 1:A:120:ARG:HB2 | 1:B:111:HIS:H    | 2        | 0.26          |
| (1,1760) | 1:A:120:ARG:HB3 | 1:B:111:HIS:H    | 2        | 0.26          |
| (1,175)  | 1:A:83:HIS:HA   | 1:A:83:HIS:HB3   | 4        | 0.26          |
| (1,175)  | 1:A:83:HIS:HA   | 1:A:83:HIS:HB3   | 6        | 0.26          |
| (1,174)  | 1:A:83:HIS:HA   | 1:A:83:HIS:HB3   | 4        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,174)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB3   | 6        | 0.26          |
| (1,1721) | 1:B:148:PRO:HB2  | 1:B:149:ARG:H    | 7        | 0.26          |
| (1,1721) | 1:B:148:PRO:HB3  | 1:B:149:ARG:H    | 7        | 0.26          |
| (1,1694) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA    | 4        | 0.26          |
| (1,1693) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA    | 4        | 0.26          |
| (1,1684) | 1:B:145:VAL:HB   | 1:B:145:VAL:H    | 6        | 0.26          |
| (1,1652) | 1:B:142:VAL:HG11 | 1:B:143:LEU:H    | 6        | 0.26          |
| (1,1652) | 1:B:142:VAL:HG12 | 1:B:143:LEU:H    | 6        | 0.26          |
| (1,1652) | 1:B:142:VAL:HG13 | 1:B:143:LEU:H    | 6        | 0.26          |
| (1,1652) | 1:B:142:VAL:HG21 | 1:B:143:LEU:H    | 6        | 0.26          |
| (1,1652) | 1:B:142:VAL:HG22 | 1:B:143:LEU:H    | 6        | 0.26          |
| (1,1652) | 1:B:142:VAL:HG23 | 1:B:143:LEU:H    | 6        | 0.26          |
| (1,1638) | 1:B:141:GLY:HA2  | 1:B:141:GLY:H    | 6        | 0.26          |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB2  | 3        | 0.26          |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB3  | 3        | 0.26          |
| (1,160)  | 1:A:81:VAL:H     | 1:A:82:LYS:H     | 1        | 0.26          |
| (1,1596) | 1:B:134:THR:H    | 1:B:134:THR:HG21 | 7        | 0.26          |
| (1,1596) | 1:B:134:THR:H    | 1:B:134:THR:HG22 | 7        | 0.26          |
| (1,1596) | 1:B:134:THR:H    | 1:B:134:THR:HG23 | 7        | 0.26          |
| (1,159)  | 1:A:81:VAL:H     | 1:A:82:LYS:H     | 1        | 0.26          |
| (1,1553) | 1:B:129:ASP:H    | 1:B:132:THR:HG1  | 7        | 0.26          |
| (1,1517) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HB   | 3        | 0.26          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD11 | 3        | 0.26          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD12 | 3        | 0.26          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD13 | 3        | 0.26          |
| (1,1476) | 1:B:123:ARG:HA   | 1:B:123:ARG:HD2  | 5        | 0.26          |
| (1,1476) | 1:B:123:ARG:HA   | 1:B:123:ARG:HD3  | 5        | 0.26          |
| (1,1467) | 1:B:122:TYR:HA   | 1:B:123:ARG:HB3  | 8        | 0.26          |
| (1,1460) | 1:B:122:TYR:HB2  | 1:B:122:TYR:HA   | 2        | 0.26          |
| (1,1460) | 1:B:122:TYR:HB3  | 1:B:122:TYR:HA   | 2        | 0.26          |
| (1,1458) | 1:B:122:TYR:HB2  | 1:B:122:TYR:HA   | 2        | 0.26          |
| (1,1458) | 1:B:122:TYR:HB3  | 1:B:122:TYR:HA   | 2        | 0.26          |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD11  | 9        | 0.26          |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD12  | 9        | 0.26          |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD13  | 9        | 0.26          |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD11  | 9        | 0.26          |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD12  | 9        | 0.26          |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD13  | 9        | 0.26          |
| (1,1446) | 1:B:119:HIS:H    | 1:B:120:ARG:H    | 5        | 0.26          |
| (1,1443) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA   | 2        | 0.26          |
| (1,1442) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA   | 2        | 0.26          |
| (1,1417) | 1:B:118:PHE:HE1  | 1:B:102:GLY:H    | 7        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1417) | 1:B:118:PHE:HE2 | 1:B:102:GLY:H   | 7        | 0.26          |
| (1,1413) | 1:B:117:GLU:HA  | 1:B:117:GLU:H   | 7        | 0.26          |
| (1,138)  | 1:A:79:LEU:HD11 | 1:A:79:LEU:HA   | 4        | 0.26          |
| (1,138)  | 1:A:79:LEU:HD12 | 1:A:79:LEU:HA   | 4        | 0.26          |
| (1,138)  | 1:A:79:LEU:HD13 | 1:A:79:LEU:HA   | 4        | 0.26          |
| (1,138)  | 1:A:79:LEU:HD21 | 1:A:79:LEU:HA   | 4        | 0.26          |
| (1,138)  | 1:A:79:LEU:HD22 | 1:A:79:LEU:HA   | 4        | 0.26          |
| (1,138)  | 1:A:79:LEU:HD23 | 1:A:79:LEU:HA   | 4        | 0.26          |
| (1,1354) | 1:B:113:PHE:H   | 1:B:112:GLY:H   | 2        | 0.26          |
| (1,1336) | 1:B:111:HIS:HB2 | 1:B:112:GLY:H   | 2        | 0.26          |
| (1,1314) | 1:B:109:ASP:H   | 1:B:109:ASP:HB2 | 5        | 0.26          |
| (1,1314) | 1:B:109:ASP:H   | 1:B:109:ASP:HB3 | 5        | 0.26          |
| (1,129)  | 1:A:78:ASN:HB3  | 1:A:79:LEU:H    | 4        | 0.26          |
| (1,1278) | 1:B:105:GLU:HB2 | 1:B:105:GLU:H   | 2        | 0.26          |
| (1,1278) | 1:B:105:GLU:HB3 | 1:B:105:GLU:H   | 2        | 0.26          |
| (1,1272) | 1:B:104:HIS:HB3 | 1:B:104:HIS:HA  | 3        | 0.26          |
| (1,1271) | 1:B:104:HIS:HB3 | 1:B:104:HIS:HA  | 3        | 0.26          |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD11 | 9        | 0.26          |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD12 | 9        | 0.26          |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD13 | 9        | 0.26          |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD21 | 9        | 0.26          |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD22 | 9        | 0.26          |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD23 | 9        | 0.26          |
| (1,1257) | 1:B:102:GLY:HA2 | 1:B:103:LYS:H   | 9        | 0.26          |
| (1,1227) | 1:B:100:VAL:HA  | 1:B:100:VAL:H   | 5        | 0.26          |
| (1,1168) | 1:B:95:GLY:H    | 1:B:94:LEU:HG   | 8        | 0.26          |
| (1,1156) | 1:B:94:LEU:H    | 1:B:93:VAL:HB   | 2        | 0.26          |
| (1,1156) | 1:B:94:LEU:H    | 1:B:93:VAL:HB   | 6        | 0.26          |
| (1,1156) | 1:B:94:LEU:H    | 1:B:93:VAL:HB   | 9        | 0.26          |
| (1,1152) | 1:B:93:VAL:HG11 | 1:B:93:VAL:H    | 8        | 0.26          |
| (1,1152) | 1:B:93:VAL:HG12 | 1:B:93:VAL:H    | 8        | 0.26          |
| (1,1152) | 1:B:93:VAL:HG13 | 1:B:93:VAL:H    | 8        | 0.26          |
| (1,1152) | 1:B:93:VAL:HG21 | 1:B:93:VAL:H    | 8        | 0.26          |
| (1,1152) | 1:B:93:VAL:HG22 | 1:B:93:VAL:H    | 8        | 0.26          |
| (1,1152) | 1:B:93:VAL:HG23 | 1:B:93:VAL:H    | 8        | 0.26          |
| (1,1148) | 1:B:92:LYS:H    | 1:B:101:HIS:H   | 3        | 0.26          |
| (1,1145) | 1:B:92:LYS:H    | 1:B:93:VAL:H    | 6        | 0.26          |
| (1,1139) | 1:B:92:LYS:H    | 1:B:91:VAL:HA   | 7        | 0.26          |
| (1,1120) | 1:B:89:LEU:HA   | 1:B:90:LYS:H    | 1        | 0.26          |
| (1,1120) | 1:B:89:LEU:HA   | 1:B:90:LYS:H    | 4        | 0.26          |
| (1,1085) | 1:B:86:PRO:HB2  | 1:B:85:SER:HA   | 4        | 0.26          |
| (1,1085) | 1:B:86:PRO:HB3  | 1:B:85:SER:HA   | 4        | 0.26          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1042) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3  | 4        | 0.26          |
| (1,1042) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3  | 6        | 0.26          |
| (1,1041) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3  | 4        | 0.26          |
| (1,1041) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3  | 6        | 0.26          |
| (1,1027) | 1:B:81:VAL:H     | 1:B:82:LYS:H    | 1        | 0.26          |
| (1,1026) | 1:B:81:VAL:H     | 1:B:82:LYS:H    | 1        | 0.26          |
| (1,1005) | 1:B:79:LEU:HD11  | 1:B:79:LEU:HA   | 4        | 0.26          |
| (1,1005) | 1:B:79:LEU:HD12  | 1:B:79:LEU:HA   | 4        | 0.26          |
| (1,1005) | 1:B:79:LEU:HD13  | 1:B:79:LEU:HA   | 4        | 0.26          |
| (1,1005) | 1:B:79:LEU:HD21  | 1:B:79:LEU:HA   | 4        | 0.26          |
| (1,1005) | 1:B:79:LEU:HD22  | 1:B:79:LEU:HA   | 4        | 0.26          |
| (1,1005) | 1:B:79:LEU:HD23  | 1:B:79:LEU:HA   | 4        | 0.26          |
| (1,995)  | 1:B:78:ASN:HA    | 1:B:79:LEU:H    | 1        | 0.25          |
| (1,987)  | 1:B:78:ASN:HA    | 1:B:78:ASN:HB3  | 7        | 0.25          |
| (1,964)  | 1:B:77:VAL:HG21  | 1:B:77:VAL:H    | 1        | 0.25          |
| (1,964)  | 1:B:77:VAL:HG22  | 1:B:77:VAL:H    | 1        | 0.25          |
| (1,964)  | 1:B:77:VAL:HG23  | 1:B:77:VAL:H    | 1        | 0.25          |
| (1,940)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2 | 8        | 0.25          |
| (1,937)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2 | 8        | 0.25          |
| (1,934)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2 | 8        | 0.25          |
| (1,898)  | 1:B:73:ASP:H     | 1:B:72:LYS:HB2  | 8        | 0.25          |
| (1,898)  | 1:B:73:ASP:H     | 1:B:72:LYS:HB3  | 8        | 0.25          |
| (1,895)  | 1:B:72:LYS:H     | 1:B:72:LYS:HA   | 8        | 0.25          |
| (1,854)  | 1:A:148:PRO:HB2  | 1:A:149:ARG:H   | 5        | 0.25          |
| (1,854)  | 1:A:148:PRO:HB3  | 1:A:149:ARG:H   | 5        | 0.25          |
| (1,811)  | 1:A:145:VAL:HB   | 1:A:77:VAL:HB   | 3        | 0.25          |
| (1,810)  | 1:A:144:THR:HG21 | 1:A:146:ASP:HB2 | 1        | 0.25          |
| (1,810)  | 1:A:144:THR:HG22 | 1:A:146:ASP:HB2 | 1        | 0.25          |
| (1,810)  | 1:A:144:THR:HG23 | 1:A:146:ASP:HB2 | 1        | 0.25          |
| (1,809)  | 1:A:144:THR:HG21 | 1:A:146:ASP:HB3 | 6        | 0.25          |
| (1,809)  | 1:A:144:THR:HG22 | 1:A:146:ASP:HB3 | 6        | 0.25          |
| (1,809)  | 1:A:144:THR:HG23 | 1:A:146:ASP:HB3 | 6        | 0.25          |
| (1,771)  | 1:A:141:GLY:HA2  | 1:A:141:GLY:H   | 7        | 0.25          |
| (1,770)  | 1:A:141:GLY:H    | 1:A:140:ASP:H   | 4        | 0.25          |
| (1,768)  | 1:A:141:GLY:H    | 1:A:140:ASP:H   | 4        | 0.25          |
| (1,749)  | 1:A:136:SER:HA   | 1:A:137:LEU:H   | 6        | 0.25          |
| (1,745)  | 1:A:136:SER:H    | 1:A:135:SER:H   | 1        | 0.25          |
| (1,73)   | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2 | 8        | 0.25          |
| (1,728)  | 1:A:133:ILE:HG12 | 1:A:147:GLY:HA2 | 7        | 0.25          |
| (1,728)  | 1:A:133:ILE:HG13 | 1:A:147:GLY:HA2 | 7        | 0.25          |
| (1,70)   | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2 | 8        | 0.25          |
| (1,67)   | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2 | 8        | 0.25          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,614) | 1:A:124:ILE:HD11 | 1:A:96:ASP:H    | 4        | 0.25          |
| (1,614) | 1:A:124:ILE:HD12 | 1:A:96:ASP:H    | 4        | 0.25          |
| (1,614) | 1:A:124:ILE:HD13 | 1:A:96:ASP:H    | 4        | 0.25          |
| (1,595) | 1:A:122:TYR:HD1  | 1:A:122:TYR:H   | 6        | 0.25          |
| (1,595) | 1:A:122:TYR:HD2  | 1:A:122:TYR:H   | 6        | 0.25          |
| (1,590) | 1:A:122:TYR:HA   | 1:A:98:ILE:H    | 9        | 0.25          |
| (1,588) | 1:A:122:TYR:HB2  | 1:A:98:ILE:HD11 | 5        | 0.25          |
| (1,588) | 1:A:122:TYR:HB2  | 1:A:98:ILE:HD12 | 5        | 0.25          |
| (1,588) | 1:A:122:TYR:HB2  | 1:A:98:ILE:HD13 | 5        | 0.25          |
| (1,588) | 1:A:122:TYR:HB3  | 1:A:98:ILE:HD11 | 5        | 0.25          |
| (1,588) | 1:A:122:TYR:HB3  | 1:A:98:ILE:HD12 | 5        | 0.25          |
| (1,588) | 1:A:122:TYR:HB3  | 1:A:98:ILE:HD13 | 5        | 0.25          |
| (1,546) | 1:A:117:GLU:HA   | 1:A:117:GLU:H   | 1        | 0.25          |
| (1,546) | 1:A:117:GLU:HA   | 1:A:117:GLU:H   | 5        | 0.25          |
| (1,494) | 1:A:113:PHE:HA   | 1:A:113:PHE:HD1 | 4        | 0.25          |
| (1,494) | 1:A:113:PHE:HA   | 1:A:113:PHE:HD2 | 4        | 0.25          |
| (1,485) | 1:A:113:PHE:HA   | 1:A:108:GLN:HA  | 7        | 0.25          |
| (1,470) | 1:A:111:HIS:HA   | 1:A:112:GLY:H   | 5        | 0.25          |
| (1,445) | 1:A:108:GLN:HA   | 1:A:113:PHE:H   | 4        | 0.25          |
| (1,430) | 1:A:107:ARG:H    | 1:A:108:GLN:H   | 6        | 0.25          |
| (1,414) | 1:A:105:GLU:HG2  | 1:A:105:GLU:H   | 2        | 0.25          |
| (1,414) | 1:A:105:GLU:HG3  | 1:A:105:GLU:H   | 2        | 0.25          |
| (1,413) | 1:A:105:GLU:HG2  | 1:A:105:GLU:H   | 2        | 0.25          |
| (1,413) | 1:A:105:GLU:HG3  | 1:A:105:GLU:H   | 2        | 0.25          |
| (1,411) | 1:A:105:GLU:HB2  | 1:A:105:GLU:H   | 2        | 0.25          |
| (1,411) | 1:A:105:GLU:HB3  | 1:A:105:GLU:H   | 2        | 0.25          |
| (1,407) | 1:A:104:HIS:HA   | 1:A:105:GLU:H   | 3        | 0.25          |
| (1,395) | 1:A:103:LYS:HG2  | 1:A:103:LYS:H   | 9        | 0.25          |
| (1,395) | 1:A:103:LYS:HG3  | 1:A:103:LYS:H   | 9        | 0.25          |
| (1,360) | 1:A:100:VAL:HA   | 1:A:100:VAL:H   | 7        | 0.25          |
| (1,351) | 1:A:99:GLU:HA    | 1:A:99:GLU:H    | 3        | 0.25          |
| (1,314) | 1:A:96:ASP:HB2   | 1:A:96:ASP:H    | 6        | 0.25          |
| (1,314) | 1:A:96:ASP:HB3   | 1:A:96:ASP:H    | 6        | 0.25          |
| (1,313) | 1:A:96:ASP:HB2   | 1:A:96:ASP:H    | 6        | 0.25          |
| (1,313) | 1:A:96:ASP:HB3   | 1:A:96:ASP:H    | 6        | 0.25          |
| (1,311) | 1:A:96:ASP:HB2   | 1:A:96:ASP:H    | 6        | 0.25          |
| (1,311) | 1:A:96:ASP:HB3   | 1:A:96:ASP:H    | 6        | 0.25          |
| (1,31)  | 1:A:73:ASP:H     | 1:A:72:LYS:HB2  | 8        | 0.25          |
| (1,31)  | 1:A:73:ASP:H     | 1:A:72:LYS:HB3  | 8        | 0.25          |
| (1,305) | 1:A:95:GLY:HA2   | 1:A:96:ASP:H    | 4        | 0.25          |
| (1,305) | 1:A:95:GLY:HA2   | 1:A:96:ASP:H    | 5        | 0.25          |
| (1,285) | 1:A:93:VAL:HG11  | 1:A:93:VAL:H    | 8        | 0.25          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,285)  | 1:A:93:VAL:HG12  | 1:A:93:VAL:H    | 8        | 0.25          |
| (1,285)  | 1:A:93:VAL:HG13  | 1:A:93:VAL:H    | 8        | 0.25          |
| (1,285)  | 1:A:93:VAL:HG21  | 1:A:93:VAL:H    | 8        | 0.25          |
| (1,285)  | 1:A:93:VAL:HG22  | 1:A:93:VAL:H    | 8        | 0.25          |
| (1,285)  | 1:A:93:VAL:HG23  | 1:A:93:VAL:H    | 8        | 0.25          |
| (1,28)   | 1:A:72:LYS:H     | 1:A:72:LYS:HA   | 8        | 0.25          |
| (1,278)  | 1:A:92:LYS:H     | 1:A:93:VAL:H    | 9        | 0.25          |
| (1,272)  | 1:A:92:LYS:H     | 1:A:91:VAL:HA   | 6        | 0.25          |
| (1,272)  | 1:A:92:LYS:H     | 1:A:91:VAL:HA   | 8        | 0.25          |
| (1,267)  | 1:A:90:LYS:HB2   | 1:A:101:HIS:HB3 | 6        | 0.25          |
| (1,267)  | 1:A:90:LYS:HB3   | 1:A:101:HIS:HB3 | 6        | 0.25          |
| (1,253)  | 1:A:89:LEU:HA    | 1:A:90:LYS:H    | 4        | 0.25          |
| (1,253)  | 1:A:89:LEU:HA    | 1:A:90:LYS:H    | 9        | 0.25          |
| (1,242)  | 1:A:89:LEU:H     | 1:A:88:GLU:H    | 4        | 0.25          |
| (1,241)  | 1:A:89:LEU:H     | 1:A:88:GLU:H    | 4        | 0.25          |
| (1,226)  | 1:A:87:GLU:HG2   | 1:A:88:GLU:H    | 1        | 0.25          |
| (1,226)  | 1:A:87:GLU:HG3   | 1:A:88:GLU:H    | 1        | 0.25          |
| (1,216)  | 1:A:85:SER:HB2   | 1:A:89:LEU:H    | 2        | 0.25          |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG2  | 2        | 0.25          |
| (1,210)  | 1:A:85:SER:HB2   | 1:A:87:GLU:HG3  | 2        | 0.25          |
| (1,199)  | 1:A:84:PHE:HB2   | 1:A:85:SER:H    | 8        | 0.25          |
| (1,199)  | 1:A:84:PHE:HB3   | 1:A:85:SER:H    | 8        | 0.25          |
| (1,185)  | 1:A:83:HIS:HB3   | 1:A:104:HIS:HB2 | 2        | 0.25          |
| (1,1721) | 1:B:148:PRO:HB2  | 1:B:149:ARG:H   | 5        | 0.25          |
| (1,1721) | 1:B:148:PRO:HB3  | 1:B:149:ARG:H   | 5        | 0.25          |
| (1,1678) | 1:B:145:VAL:HB   | 1:B:77:VAL:HB   | 3        | 0.25          |
| (1,1677) | 1:B:144:THR:HG21 | 1:B:146:ASP:HB2 | 1        | 0.25          |
| (1,1677) | 1:B:144:THR:HG22 | 1:B:146:ASP:HB2 | 1        | 0.25          |
| (1,1677) | 1:B:144:THR:HG23 | 1:B:146:ASP:HB2 | 1        | 0.25          |
| (1,1676) | 1:B:144:THR:HG21 | 1:B:146:ASP:HB3 | 6        | 0.25          |
| (1,1676) | 1:B:144:THR:HG22 | 1:B:146:ASP:HB3 | 6        | 0.25          |
| (1,1676) | 1:B:144:THR:HG23 | 1:B:146:ASP:HB3 | 6        | 0.25          |
| (1,1675) | 1:B:144:THR:H    | 1:B:145:VAL:H   | 8        | 0.25          |
| (1,1670) | 1:B:144:THR:H    | 1:B:145:VAL:H   | 8        | 0.25          |
| (1,1638) | 1:B:141:GLY:HA2  | 1:B:141:GLY:H   | 7        | 0.25          |
| (1,1637) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 4        | 0.25          |
| (1,1635) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 4        | 0.25          |
| (1,1616) | 1:B:136:SER:HA   | 1:B:137:LEU:H   | 6        | 0.25          |
| (1,1612) | 1:B:136:SER:H    | 1:B:135:SER:H   | 1        | 0.25          |
| (1,1595) | 1:B:133:ILE:HG12 | 1:B:147:GLY:HA2 | 7        | 0.25          |
| (1,1595) | 1:B:133:ILE:HG13 | 1:B:147:GLY:HA2 | 7        | 0.25          |
| (1,1462) | 1:B:122:TYR:HD1  | 1:B:122:TYR:H   | 6        | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1462) | 1:B:122:TYR:HD2 | 1:B:122:TYR:H   | 6        | 0.25          |
| (1,1457) | 1:B:122:TYR:HA  | 1:B:98:ILE:H    | 9        | 0.25          |
| (1,1413) | 1:B:117:GLU:HA  | 1:B:117:GLU:H   | 1        | 0.25          |
| (1,138)  | 1:A:79:LEU:HD11 | 1:A:79:LEU:HA   | 3        | 0.25          |
| (1,138)  | 1:A:79:LEU:HD12 | 1:A:79:LEU:HA   | 3        | 0.25          |
| (1,138)  | 1:A:79:LEU:HD13 | 1:A:79:LEU:HA   | 3        | 0.25          |
| (1,138)  | 1:A:79:LEU:HD21 | 1:A:79:LEU:HA   | 3        | 0.25          |
| (1,138)  | 1:A:79:LEU:HD22 | 1:A:79:LEU:HA   | 3        | 0.25          |
| (1,138)  | 1:A:79:LEU:HD23 | 1:A:79:LEU:HA   | 3        | 0.25          |
| (1,1352) | 1:B:113:PHE:HA  | 1:B:108:GLN:HA  | 7        | 0.25          |
| (1,1312) | 1:B:108:GLN:HA  | 1:B:113:PHE:H   | 4        | 0.25          |
| (1,1297) | 1:B:107:ARG:H   | 1:B:108:GLN:H   | 6        | 0.25          |
| (1,1281) | 1:B:105:GLU:HG2 | 1:B:105:GLU:H   | 2        | 0.25          |
| (1,1281) | 1:B:105:GLU:HG3 | 1:B:105:GLU:H   | 2        | 0.25          |
| (1,1280) | 1:B:105:GLU:HG2 | 1:B:105:GLU:H   | 2        | 0.25          |
| (1,1280) | 1:B:105:GLU:HG3 | 1:B:105:GLU:H   | 2        | 0.25          |
| (1,128)  | 1:A:78:ASN:HA   | 1:A:79:LEU:H    | 1        | 0.25          |
| (1,1274) | 1:B:104:HIS:HA  | 1:B:105:GLU:H   | 3        | 0.25          |
| (1,1262) | 1:B:103:LYS:HG2 | 1:B:103:LYS:H   | 9        | 0.25          |
| (1,1262) | 1:B:103:LYS:HG3 | 1:B:103:LYS:H   | 9        | 0.25          |
| (1,1227) | 1:B:100:VAL:HA  | 1:B:100:VAL:H   | 7        | 0.25          |
| (1,120)  | 1:A:78:ASN:HA   | 1:A:78:ASN:HB3  | 7        | 0.25          |
| (1,1181) | 1:B:96:ASP:HB2  | 1:B:96:ASP:H    | 6        | 0.25          |
| (1,1181) | 1:B:96:ASP:HB3  | 1:B:96:ASP:H    | 6        | 0.25          |
| (1,1180) | 1:B:96:ASP:HB2  | 1:B:96:ASP:H    | 6        | 0.25          |
| (1,1180) | 1:B:96:ASP:HB3  | 1:B:96:ASP:H    | 6        | 0.25          |
| (1,1178) | 1:B:96:ASP:HB2  | 1:B:96:ASP:H    | 6        | 0.25          |
| (1,1178) | 1:B:96:ASP:HB3  | 1:B:96:ASP:H    | 6        | 0.25          |
| (1,1172) | 1:B:95:GLY:HA2  | 1:B:96:ASP:H    | 4        | 0.25          |
| (1,1172) | 1:B:95:GLY:HA2  | 1:B:96:ASP:H    | 5        | 0.25          |
| (1,1145) | 1:B:92:LYS:H    | 1:B:93:VAL:H    | 9        | 0.25          |
| (1,1139) | 1:B:92:LYS:H    | 1:B:91:VAL:HA   | 6        | 0.25          |
| (1,1139) | 1:B:92:LYS:H    | 1:B:91:VAL:HA   | 8        | 0.25          |
| (1,1134) | 1:B:90:LYS:HB2  | 1:B:101:HIS:HB3 | 6        | 0.25          |
| (1,1134) | 1:B:90:LYS:HB3  | 1:B:101:HIS:HB3 | 6        | 0.25          |
| (1,1120) | 1:B:89:LEU:HA   | 1:B:90:LYS:H    | 9        | 0.25          |
| (1,1109) | 1:B:89:LEU:H    | 1:B:88:GLU:H    | 4        | 0.25          |
| (1,1108) | 1:B:89:LEU:H    | 1:B:88:GLU:H    | 4        | 0.25          |
| (1,1093) | 1:B:87:GLU:HG2  | 1:B:88:GLU:H    | 1        | 0.25          |
| (1,1093) | 1:B:87:GLU:HG3  | 1:B:88:GLU:H    | 1        | 0.25          |
| (1,1083) | 1:B:85:SER:HB2  | 1:B:89:LEU:H    | 2        | 0.25          |
| (1,1077) | 1:B:85:SER:HB2  | 1:B:87:GLU:HG2  | 2        | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1077) | 1:B:85:SER:HB2   | 1:B:87:GLU:HG3   | 2        | 0.25          |
| (1,1052) | 1:B:83:HIS:HB3   | 1:B:104:HIS:HB2  | 2        | 0.25          |
| (1,105)  | 1:A:77:VAL:HG21  | 1:A:79:LEU:HG    | 6        | 0.25          |
| (1,105)  | 1:A:77:VAL:HG22  | 1:A:79:LEU:HG    | 6        | 0.25          |
| (1,105)  | 1:A:77:VAL:HG23  | 1:A:79:LEU:HG    | 6        | 0.25          |
| (1,1005) | 1:B:79:LEU:HD11  | 1:B:79:LEU:HA    | 3        | 0.25          |
| (1,1005) | 1:B:79:LEU:HD12  | 1:B:79:LEU:HA    | 3        | 0.25          |
| (1,1005) | 1:B:79:LEU:HD13  | 1:B:79:LEU:HA    | 3        | 0.25          |
| (1,1005) | 1:B:79:LEU:HD21  | 1:B:79:LEU:HA    | 3        | 0.25          |
| (1,1005) | 1:B:79:LEU:HD22  | 1:B:79:LEU:HA    | 3        | 0.25          |
| (1,1005) | 1:B:79:LEU:HD23  | 1:B:79:LEU:HA    | 3        | 0.25          |
| (1,987)  | 1:B:78:ASN:HA    | 1:B:78:ASN:HB3   | 8        | 0.24          |
| (1,974)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:HG    | 6        | 0.24          |
| (1,974)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:HG    | 6        | 0.24          |
| (1,974)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:HG    | 6        | 0.24          |
| (1,942)  | 1:B:76:SER:HB3   | 1:B:146:ASP:HB3  | 1        | 0.24          |
| (1,898)  | 1:B:73:ASP:H     | 1:B:72:LYS:HB2   | 1        | 0.24          |
| (1,898)  | 1:B:73:ASP:H     | 1:B:72:LYS:HB3   | 1        | 0.24          |
| (1,870)  | 1:B:66:SER:HB2   | 1:B:66:SER:H     | 2        | 0.24          |
| (1,847)  | 1:A:147:GLY:HA2  | 1:A:147:GLY:H    | 4        | 0.24          |
| (1,814)  | 1:A:145:VAL:HG11 | 1:A:135:SER:H    | 3        | 0.24          |
| (1,814)  | 1:A:145:VAL:HG12 | 1:A:135:SER:H    | 3        | 0.24          |
| (1,814)  | 1:A:145:VAL:HG13 | 1:A:135:SER:H    | 3        | 0.24          |
| (1,812)  | 1:A:145:VAL:HB   | 1:A:135:SER:HA   | 2        | 0.24          |
| (1,811)  | 1:A:145:VAL:HB   | 1:A:77:VAL:HB    | 4        | 0.24          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD11 | 9        | 0.24          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD12 | 9        | 0.24          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD13 | 9        | 0.24          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD21 | 9        | 0.24          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD22 | 9        | 0.24          |
| (1,798)  | 1:A:144:THR:H    | 1:A:143:LEU:HD23 | 9        | 0.24          |
| (1,771)  | 1:A:141:GLY:HA2  | 1:A:141:GLY:H    | 5        | 0.24          |
| (1,771)  | 1:A:141:GLY:HA2  | 1:A:141:GLY:H    | 9        | 0.24          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD11 | 6        | 0.24          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD12 | 6        | 0.24          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD13 | 6        | 0.24          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD21 | 6        | 0.24          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD22 | 6        | 0.24          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD23 | 6        | 0.24          |
| (1,75)   | 1:A:76:SER:HB3   | 1:A:146:ASP:HB3  | 1        | 0.24          |
| (1,715)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HG2  | 9        | 0.24          |
| (1,715)  | 1:A:133:ILE:HD11 | 1:A:130:PRO:HG3  | 9        | 0.24          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,715) | 1:A:133:ILE:HD12 | 1:A:130:PRO:HG2 | 9        | 0.24          |
| (1,715) | 1:A:133:ILE:HD12 | 1:A:130:PRO:HG3 | 9        | 0.24          |
| (1,715) | 1:A:133:ILE:HD13 | 1:A:130:PRO:HG2 | 9        | 0.24          |
| (1,715) | 1:A:133:ILE:HD13 | 1:A:130:PRO:HG3 | 9        | 0.24          |
| (1,592) | 1:A:122:TYR:HA   | 1:A:122:TYR:HD1 | 2        | 0.24          |
| (1,592) | 1:A:122:TYR:HA   | 1:A:122:TYR:HD2 | 2        | 0.24          |
| (1,569) | 1:A:119:HIS:HA   | 1:A:101:HIS:HA  | 6        | 0.24          |
| (1,502) | 1:A:114:ILE:HD11 | 1:A:104:HIS:HB2 | 7        | 0.24          |
| (1,502) | 1:A:114:ILE:HD12 | 1:A:104:HIS:HB2 | 7        | 0.24          |
| (1,502) | 1:A:114:ILE:HD13 | 1:A:104:HIS:HB2 | 7        | 0.24          |
| (1,470) | 1:A:111:HIS:HA   | 1:A:112:GLY:H   | 7        | 0.24          |
| (1,427) | 1:A:107:ARG:HB3  | 1:A:107:ARG:H   | 9        | 0.24          |
| (1,415) | 1:A:105:GLU:HA   | 1:A:106:GLU:H   | 8        | 0.24          |
| (1,369) | 1:A:101:HIS:H    | 1:A:100:VAL:HA  | 6        | 0.24          |
| (1,369) | 1:A:101:HIS:H    | 1:A:100:VAL:HA  | 9        | 0.24          |
| (1,360) | 1:A:100:VAL:HA   | 1:A:100:VAL:H   | 4        | 0.24          |
| (1,355) | 1:A:99:GLU:HB2   | 1:A:121:LYS:HG2 | 7        | 0.24          |
| (1,355) | 1:A:99:GLU:HB2   | 1:A:121:LYS:HG3 | 7        | 0.24          |
| (1,355) | 1:A:99:GLU:HB3   | 1:A:121:LYS:HG2 | 7        | 0.24          |
| (1,355) | 1:A:99:GLU:HB3   | 1:A:121:LYS:HG3 | 7        | 0.24          |
| (1,351) | 1:A:99:GLU:HA    | 1:A:99:GLU:H    | 2        | 0.24          |
| (1,351) | 1:A:99:GLU:HA    | 1:A:99:GLU:H    | 6        | 0.24          |
| (1,346) | 1:A:98:ILE:H     | 1:A:122:TYR:H   | 5        | 0.24          |
| (1,346) | 1:A:98:ILE:H     | 1:A:122:TYR:H   | 6        | 0.24          |
| (1,345) | 1:A:98:ILE:H     | 1:A:122:TYR:H   | 5        | 0.24          |
| (1,345) | 1:A:98:ILE:H     | 1:A:122:TYR:H   | 6        | 0.24          |
| (1,320) | 1:A:96:ASP:HA    | 1:A:124:ILE:H   | 5        | 0.24          |
| (1,31)  | 1:A:73:ASP:H     | 1:A:72:LYS:HB2  | 1        | 0.24          |
| (1,31)  | 1:A:73:ASP:H     | 1:A:72:LYS:HB3  | 1        | 0.24          |
| (1,305) | 1:A:95:GLY:HA2   | 1:A:96:ASP:H    | 1        | 0.24          |
| (1,305) | 1:A:95:GLY:HA2   | 1:A:96:ASP:H    | 2        | 0.24          |
| (1,305) | 1:A:95:GLY:HA2   | 1:A:96:ASP:H    | 6        | 0.24          |
| (1,305) | 1:A:95:GLY:HA2   | 1:A:96:ASP:H    | 7        | 0.24          |
| (1,305) | 1:A:95:GLY:HA2   | 1:A:96:ASP:H    | 9        | 0.24          |
| (1,3)   | 1:A:66:SER:HB2   | 1:A:66:SER:H    | 2        | 0.24          |
| (1,299) | 1:A:95:GLY:HA3   | 1:A:94:LEU:HD11 | 3        | 0.24          |
| (1,299) | 1:A:95:GLY:HA3   | 1:A:94:LEU:HD12 | 3        | 0.24          |
| (1,299) | 1:A:95:GLY:HA3   | 1:A:94:LEU:HD13 | 3        | 0.24          |
| (1,299) | 1:A:95:GLY:HA3   | 1:A:94:LEU:HD21 | 3        | 0.24          |
| (1,299) | 1:A:95:GLY:HA3   | 1:A:94:LEU:HD22 | 3        | 0.24          |
| (1,299) | 1:A:95:GLY:HA3   | 1:A:94:LEU:HD23 | 3        | 0.24          |
| (1,289) | 1:A:94:LEU:H     | 1:A:93:VAL:HB   | 4        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,278)  | 1:A:92:LYS:H     | 1:A:93:VAL:H     | 5        | 0.24          |
| (1,276)  | 1:A:92:LYS:H     | 1:A:92:LYS:HA    | 4        | 0.24          |
| (1,275)  | 1:A:92:LYS:H     | 1:A:92:LYS:HG2   | 8        | 0.24          |
| (1,275)  | 1:A:92:LYS:H     | 1:A:92:LYS:HG3   | 8        | 0.24          |
| (1,272)  | 1:A:92:LYS:H     | 1:A:91:VAL:HA    | 2        | 0.24          |
| (1,267)  | 1:A:90:LYS:HB2   | 1:A:101:HIS:HB3  | 7        | 0.24          |
| (1,267)  | 1:A:90:LYS:HB3   | 1:A:101:HIS:HB3  | 7        | 0.24          |
| (1,266)  | 1:A:90:LYS:HB2   | 1:A:101:HIS:HB2  | 9        | 0.24          |
| (1,266)  | 1:A:90:LYS:HB3   | 1:A:101:HIS:HB2  | 9        | 0.24          |
| (1,252)  | 1:A:89:LEU:H     | 1:A:90:LYS:H     | 6        | 0.24          |
| (1,239)  | 1:A:89:LEU:H     | 1:A:87:GLU:HA    | 7        | 0.24          |
| (1,175)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB3   | 5        | 0.24          |
| (1,174)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB3   | 5        | 0.24          |
| (1,1714) | 1:B:147:GLY:HA2  | 1:B:147:GLY:H    | 4        | 0.24          |
| (1,1681) | 1:B:145:VAL:HG11 | 1:B:135:SER:H    | 3        | 0.24          |
| (1,1681) | 1:B:145:VAL:HG12 | 1:B:135:SER:H    | 3        | 0.24          |
| (1,1681) | 1:B:145:VAL:HG13 | 1:B:135:SER:H    | 3        | 0.24          |
| (1,1679) | 1:B:145:VAL:HB   | 1:B:135:SER:HA   | 2        | 0.24          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD11 | 9        | 0.24          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD12 | 9        | 0.24          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD13 | 9        | 0.24          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD21 | 9        | 0.24          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD22 | 9        | 0.24          |
| (1,1665) | 1:B:144:THR:H    | 1:B:143:LEU:HD23 | 9        | 0.24          |
| (1,1638) | 1:B:141:GLY:HA2  | 1:B:141:GLY:H    | 5        | 0.24          |
| (1,1638) | 1:B:141:GLY:HA2  | 1:B:141:GLY:H    | 9        | 0.24          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD11 | 6        | 0.24          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD12 | 6        | 0.24          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD13 | 6        | 0.24          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD21 | 6        | 0.24          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD22 | 6        | 0.24          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD23 | 6        | 0.24          |
| (1,1582) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HG2  | 9        | 0.24          |
| (1,1582) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HG3  | 9        | 0.24          |
| (1,1582) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HG2  | 9        | 0.24          |
| (1,1582) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HG3  | 9        | 0.24          |
| (1,1582) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HG2  | 9        | 0.24          |
| (1,1582) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HG3  | 9        | 0.24          |
| (1,1481) | 1:B:124:ILE:HD11 | 1:B:96:ASP:H     | 4        | 0.24          |
| (1,1481) | 1:B:124:ILE:HD12 | 1:B:96:ASP:H     | 4        | 0.24          |
| (1,1481) | 1:B:124:ILE:HD13 | 1:B:96:ASP:H     | 4        | 0.24          |
| (1,148)  | 1:A:80:ASP:H     | 1:A:80:ASP:HB3   | 1        | 0.24          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1459) | 1:B:122:TYR:HA   | 1:B:122:TYR:HD1 | 2        | 0.24          |
| (1,1459) | 1:B:122:TYR:HA   | 1:B:122:TYR:HD2 | 2        | 0.24          |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD11 | 5        | 0.24          |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD12 | 5        | 0.24          |
| (1,1455) | 1:B:122:TYR:HB2  | 1:B:98:ILE:HD13 | 5        | 0.24          |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD11 | 5        | 0.24          |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD12 | 5        | 0.24          |
| (1,1455) | 1:B:122:TYR:HB3  | 1:B:98:ILE:HD13 | 5        | 0.24          |
| (1,1436) | 1:B:119:HIS:HA   | 1:B:101:HIS:HA  | 6        | 0.24          |
| (1,1413) | 1:B:117:GLU:HA   | 1:B:117:GLU:H   | 5        | 0.24          |
| (1,1369) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HB2 | 7        | 0.24          |
| (1,1369) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HB2 | 7        | 0.24          |
| (1,1369) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HB2 | 7        | 0.24          |
| (1,1361) | 1:B:113:PHE:HA   | 1:B:113:PHE:HD1 | 4        | 0.24          |
| (1,1361) | 1:B:113:PHE:HA   | 1:B:113:PHE:HD2 | 4        | 0.24          |
| (1,1337) | 1:B:111:HIS:HA   | 1:B:112:GLY:H   | 5        | 0.24          |
| (1,1337) | 1:B:111:HIS:HA   | 1:B:112:GLY:H   | 7        | 0.24          |
| (1,1294) | 1:B:107:ARG:HB3  | 1:B:107:ARG:H   | 9        | 0.24          |
| (1,1282) | 1:B:105:GLU:HA   | 1:B:106:GLU:H   | 8        | 0.24          |
| (1,1236) | 1:B:101:HIS:H    | 1:B:100:VAL:HA  | 6        | 0.24          |
| (1,1236) | 1:B:101:HIS:H    | 1:B:100:VAL:HA  | 9        | 0.24          |
| (1,1227) | 1:B:100:VAL:HA   | 1:B:100:VAL:H   | 4        | 0.24          |
| (1,1222) | 1:B:99:GLU:HB2   | 1:B:121:LYS:HG2 | 7        | 0.24          |
| (1,1222) | 1:B:99:GLU:HB2   | 1:B:121:LYS:HG3 | 7        | 0.24          |
| (1,1222) | 1:B:99:GLU:HB3   | 1:B:121:LYS:HG2 | 7        | 0.24          |
| (1,1222) | 1:B:99:GLU:HB3   | 1:B:121:LYS:HG3 | 7        | 0.24          |
| (1,1218) | 1:B:99:GLU:HA    | 1:B:99:GLU:H    | 2        | 0.24          |
| (1,1218) | 1:B:99:GLU:HA    | 1:B:99:GLU:H    | 3        | 0.24          |
| (1,1218) | 1:B:99:GLU:HA    | 1:B:99:GLU:H    | 6        | 0.24          |
| (1,1213) | 1:B:98:ILE:H     | 1:B:122:TYR:H   | 5        | 0.24          |
| (1,1213) | 1:B:98:ILE:H     | 1:B:122:TYR:H   | 6        | 0.24          |
| (1,1212) | 1:B:98:ILE:H     | 1:B:122:TYR:H   | 5        | 0.24          |
| (1,1212) | 1:B:98:ILE:H     | 1:B:122:TYR:H   | 6        | 0.24          |
| (1,120)  | 1:A:78:ASN:HA    | 1:A:78:ASN:HB3  | 8        | 0.24          |
| (1,1187) | 1:B:96:ASP:HA    | 1:B:124:ILE:H   | 5        | 0.24          |
| (1,1172) | 1:B:95:GLY:HA2   | 1:B:96:ASP:H    | 1        | 0.24          |
| (1,1172) | 1:B:95:GLY:HA2   | 1:B:96:ASP:H    | 6        | 0.24          |
| (1,1172) | 1:B:95:GLY:HA2   | 1:B:96:ASP:H    | 7        | 0.24          |
| (1,1172) | 1:B:95:GLY:HA2   | 1:B:96:ASP:H    | 9        | 0.24          |
| (1,1166) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HD11 | 3        | 0.24          |
| (1,1166) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HD12 | 3        | 0.24          |
| (1,1166) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HD13 | 3        | 0.24          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1166) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HD21 | 3        | 0.24          |
| (1,1166) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HD22 | 3        | 0.24          |
| (1,1166) | 1:B:95:GLY:HA3   | 1:B:94:LEU:HD23 | 3        | 0.24          |
| (1,1156) | 1:B:94:LEU:H     | 1:B:93:VAL:HB   | 4        | 0.24          |
| (1,1145) | 1:B:92:LYS:H     | 1:B:93:VAL:H    | 5        | 0.24          |
| (1,1143) | 1:B:92:LYS:H     | 1:B:92:LYS:HA   | 4        | 0.24          |
| (1,1142) | 1:B:92:LYS:H     | 1:B:92:LYS:HG2  | 8        | 0.24          |
| (1,1142) | 1:B:92:LYS:H     | 1:B:92:LYS:HG3  | 8        | 0.24          |
| (1,1139) | 1:B:92:LYS:H     | 1:B:91:VAL:HA   | 2        | 0.24          |
| (1,1134) | 1:B:90:LYS:HB2   | 1:B:101:HIS:HB3 | 7        | 0.24          |
| (1,1134) | 1:B:90:LYS:HB3   | 1:B:101:HIS:HB3 | 7        | 0.24          |
| (1,1133) | 1:B:90:LYS:HB2   | 1:B:101:HIS:HB2 | 9        | 0.24          |
| (1,1133) | 1:B:90:LYS:HB3   | 1:B:101:HIS:HB2 | 9        | 0.24          |
| (1,1119) | 1:B:89:LEU:H     | 1:B:90:LYS:H    | 6        | 0.24          |
| (1,1106) | 1:B:89:LEU:H     | 1:B:87:GLU:HA   | 7        | 0.24          |
| (1,107)  | 1:A:77:VAL:HG11  | 1:A:79:LEU:HG   | 6        | 0.24          |
| (1,107)  | 1:A:77:VAL:HG12  | 1:A:79:LEU:HG   | 6        | 0.24          |
| (1,107)  | 1:A:77:VAL:HG13  | 1:A:79:LEU:HG   | 6        | 0.24          |
| (1,1066) | 1:B:84:PHE:HB2   | 1:B:85:SER:H    | 8        | 0.24          |
| (1,1066) | 1:B:84:PHE:HB3   | 1:B:85:SER:H    | 8        | 0.24          |
| (1,1042) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3  | 5        | 0.24          |
| (1,1041) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3  | 5        | 0.24          |
| (1,1015) | 1:B:80:ASP:H     | 1:B:80:ASP:HB3  | 1        | 0.24          |
| (1,987)  | 1:B:78:ASN:HA    | 1:B:78:ASN:HB3  | 6        | 0.23          |
| (1,975)  | 1:B:77:VAL:HG11  | 1:B:79:LEU:H    | 9        | 0.23          |
| (1,975)  | 1:B:77:VAL:HG12  | 1:B:79:LEU:H    | 9        | 0.23          |
| (1,975)  | 1:B:77:VAL:HG13  | 1:B:79:LEU:H    | 9        | 0.23          |
| (1,972)  | 1:B:77:VAL:HG21  | 1:B:79:LEU:HG   | 4        | 0.23          |
| (1,972)  | 1:B:77:VAL:HG22  | 1:B:79:LEU:HG   | 4        | 0.23          |
| (1,972)  | 1:B:77:VAL:HG23  | 1:B:79:LEU:HG   | 4        | 0.23          |
| (1,945)  | 1:B:76:SER:HA    | 1:B:146:ASP:HA  | 6        | 0.23          |
| (1,941)  | 1:B:76:SER:HA    | 1:B:146:ASP:HA  | 6        | 0.23          |
| (1,909)  | 1:B:74:ARG:H     | 1:B:74:ARG:HB2  | 6        | 0.23          |
| (1,898)  | 1:B:73:ASP:H     | 1:B:72:LYS:HB2  | 7        | 0.23          |
| (1,898)  | 1:B:73:ASP:H     | 1:B:72:LYS:HB3  | 7        | 0.23          |
| (1,854)  | 1:A:148:PRO:HB2  | 1:A:149:ARG:H   | 2        | 0.23          |
| (1,854)  | 1:A:148:PRO:HB3  | 1:A:149:ARG:H   | 2        | 0.23          |
| (1,817)  | 1:A:145:VAL:HB   | 1:A:145:VAL:H   | 5        | 0.23          |
| (1,809)  | 1:A:144:THR:HG21 | 1:A:146:ASP:HB3 | 8        | 0.23          |
| (1,809)  | 1:A:144:THR:HG22 | 1:A:146:ASP:HB3 | 8        | 0.23          |
| (1,809)  | 1:A:144:THR:HG23 | 1:A:146:ASP:HB3 | 8        | 0.23          |
| (1,808)  | 1:A:144:THR:H    | 1:A:145:VAL:H   | 9        | 0.23          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,803) | 1:A:144:THR:H    | 1:A:145:VAL:H    | 9        | 0.23          |
| (1,783) | 1:A:142:VAL:HG11 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,783) | 1:A:142:VAL:HG12 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,783) | 1:A:142:VAL:HG13 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,783) | 1:A:142:VAL:HG21 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,783) | 1:A:142:VAL:HG22 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,783) | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,782) | 1:A:142:VAL:HG11 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,782) | 1:A:142:VAL:HG12 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,782) | 1:A:142:VAL:HG13 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,782) | 1:A:142:VAL:HG21 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,782) | 1:A:142:VAL:HG22 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,782) | 1:A:142:VAL:HG23 | 1:A:142:VAL:H    | 2        | 0.23          |
| (1,78)  | 1:A:76:SER:HA    | 1:A:146:ASP:HA   | 6        | 0.23          |
| (1,770) | 1:A:141:GLY:H    | 1:A:140:ASP:H    | 7        | 0.23          |
| (1,770) | 1:A:141:GLY:H    | 1:A:140:ASP:H    | 9        | 0.23          |
| (1,768) | 1:A:141:GLY:H    | 1:A:140:ASP:H    | 7        | 0.23          |
| (1,768) | 1:A:141:GLY:H    | 1:A:140:ASP:H    | 9        | 0.23          |
| (1,749) | 1:A:136:SER:HA   | 1:A:137:LEU:H    | 5        | 0.23          |
| (1,746) | 1:A:136:SER:H    | 1:A:135:SER:H    | 2        | 0.23          |
| (1,742) | 1:A:135:SER:HA   | 1:A:145:VAL:HA   | 4        | 0.23          |
| (1,740) | 1:A:135:SER:HA   | 1:A:145:VAL:HA   | 4        | 0.23          |
| (1,74)  | 1:A:76:SER:HA    | 1:A:146:ASP:HA   | 6        | 0.23          |
| (1,705) | 1:A:132:THR:HG1  | 1:A:133:ILE:H    | 5        | 0.23          |
| (1,675) | 1:A:128:VAL:H    | 1:A:126:ALA:H    | 4        | 0.23          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD11 | 8        | 0.23          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD12 | 8        | 0.23          |
| (1,647) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HD13 | 8        | 0.23          |
| (1,593) | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA   | 8        | 0.23          |
| (1,593) | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA   | 8        | 0.23          |
| (1,591) | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA   | 8        | 0.23          |
| (1,591) | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA   | 8        | 0.23          |
| (1,590) | 1:A:122:TYR:HA   | 1:A:98:ILE:H     | 8        | 0.23          |
| (1,588) | 1:A:122:TYR:HB2  | 1:A:98:ILE:HD11  | 4        | 0.23          |
| (1,588) | 1:A:122:TYR:HB2  | 1:A:98:ILE:HD12  | 4        | 0.23          |
| (1,588) | 1:A:122:TYR:HB2  | 1:A:98:ILE:HD13  | 4        | 0.23          |
| (1,588) | 1:A:122:TYR:HB3  | 1:A:98:ILE:HD11  | 4        | 0.23          |
| (1,588) | 1:A:122:TYR:HB3  | 1:A:98:ILE:HD12  | 4        | 0.23          |
| (1,588) | 1:A:122:TYR:HB3  | 1:A:98:ILE:HD13  | 4        | 0.23          |
| (1,583) | 1:A:121:LYS:HA   | 1:A:99:GLU:HA    | 8        | 0.23          |
| (1,546) | 1:A:117:GLU:HA   | 1:A:117:GLU:H    | 4        | 0.23          |
| (1,454) | 1:A:110:GLU:H    | 1:A:110:GLU:HA   | 5        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,420)  | 1:A:106:GLU:HB2 | 1:A:106:GLU:H   | 2        | 0.23          |
| (1,420)  | 1:A:106:GLU:HB3 | 1:A:106:GLU:H   | 2        | 0.23          |
| (1,42)   | 1:A:74:ARG:H    | 1:A:74:ARG:HB2  | 6        | 0.23          |
| (1,414)  | 1:A:105:GLU:HG2 | 1:A:105:GLU:H   | 9        | 0.23          |
| (1,414)  | 1:A:105:GLU:HG3 | 1:A:105:GLU:H   | 9        | 0.23          |
| (1,413)  | 1:A:105:GLU:HG2 | 1:A:105:GLU:H   | 9        | 0.23          |
| (1,413)  | 1:A:105:GLU:HG3 | 1:A:105:GLU:H   | 9        | 0.23          |
| (1,399)  | 1:A:103:LYS:HA  | 1:A:118:PHE:H   | 1        | 0.23          |
| (1,378)  | 1:A:101:HIS:HB3 | 1:A:101:HIS:H   | 7        | 0.23          |
| (1,372)  | 1:A:101:HIS:HA  | 1:A:101:HIS:HD2 | 9        | 0.23          |
| (1,360)  | 1:A:100:VAL:HA  | 1:A:100:VAL:H   | 1        | 0.23          |
| (1,360)  | 1:A:100:VAL:HA  | 1:A:100:VAL:H   | 9        | 0.23          |
| (1,339)  | 1:A:98:ILE:HB   | 1:A:98:ILE:H    | 3        | 0.23          |
| (1,339)  | 1:A:98:ILE:HB   | 1:A:98:ILE:H    | 5        | 0.23          |
| (1,330)  | 1:A:97:VAL:HA   | 1:A:123:ARG:HA  | 9        | 0.23          |
| (1,329)  | 1:A:97:VAL:HA   | 1:A:123:ARG:HA  | 9        | 0.23          |
| (1,31)   | 1:A:73:ASP:H    | 1:A:72:LYS:HB2  | 7        | 0.23          |
| (1,31)   | 1:A:73:ASP:H    | 1:A:72:LYS:HB3  | 7        | 0.23          |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD11 | 1        | 0.23          |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD12 | 1        | 0.23          |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD13 | 1        | 0.23          |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD21 | 1        | 0.23          |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD22 | 1        | 0.23          |
| (1,299)  | 1:A:95:GLY:HA3  | 1:A:94:LEU:HD23 | 1        | 0.23          |
| (1,281)  | 1:A:92:LYS:H    | 1:A:101:HIS:H   | 1        | 0.23          |
| (1,278)  | 1:A:92:LYS:H    | 1:A:93:VAL:H    | 7        | 0.23          |
| (1,272)  | 1:A:92:LYS:H    | 1:A:91:VAL:HA   | 3        | 0.23          |
| (1,272)  | 1:A:92:LYS:H    | 1:A:91:VAL:HA   | 9        | 0.23          |
| (1,252)  | 1:A:89:LEU:H    | 1:A:90:LYS:H    | 8        | 0.23          |
| (1,189)  | 1:A:84:PHE:H    | 1:A:81:VAL:HB   | 7        | 0.23          |
| (1,1770) | 1:A:123:ARG:HD2 | 1:B:113:PHE:H   | 2        | 0.23          |
| (1,1770) | 1:A:123:ARG:HD3 | 1:B:113:PHE:H   | 2        | 0.23          |
| (1,1750) | 1:A:115:SER:HB2 | 1:B:119:HIS:HE1 | 1        | 0.23          |
| (1,175)  | 1:A:83:HIS:HA   | 1:A:83:HIS:HB3  | 1        | 0.23          |
| (1,174)  | 1:A:83:HIS:HA   | 1:A:83:HIS:HB3  | 1        | 0.23          |
| (1,1721) | 1:B:148:PRO:HB2 | 1:B:149:ARG:H   | 2        | 0.23          |
| (1,1721) | 1:B:148:PRO:HB3 | 1:B:149:ARG:H   | 2        | 0.23          |
| (1,1684) | 1:B:145:VAL:HB  | 1:B:145:VAL:H   | 5        | 0.23          |
| (1,168)  | 1:A:81:VAL:HG21 | 1:A:143:LEU:HA  | 2        | 0.23          |
| (1,168)  | 1:A:81:VAL:HG22 | 1:A:143:LEU:HA  | 2        | 0.23          |
| (1,168)  | 1:A:81:VAL:HG23 | 1:A:143:LEU:HA  | 2        | 0.23          |
| (1,1678) | 1:B:145:VAL:HB  | 1:B:77:VAL:HB   | 4        | 0.23          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1676) | 1:B:144:THR:HG21 | 1:B:146:ASP:HB3 | 8        | 0.23          |
| (1,1676) | 1:B:144:THR:HG22 | 1:B:146:ASP:HB3 | 8        | 0.23          |
| (1,1676) | 1:B:144:THR:HG23 | 1:B:146:ASP:HB3 | 8        | 0.23          |
| (1,1675) | 1:B:144:THR:H    | 1:B:145:VAL:H   | 9        | 0.23          |
| (1,1670) | 1:B:144:THR:H    | 1:B:145:VAL:H   | 9        | 0.23          |
| (1,1637) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 1        | 0.23          |
| (1,1637) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 7        | 0.23          |
| (1,1637) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 9        | 0.23          |
| (1,1635) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 1        | 0.23          |
| (1,1635) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 7        | 0.23          |
| (1,1635) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 9        | 0.23          |
| (1,1616) | 1:B:136:SER:HA   | 1:B:137:LEU:H   | 5        | 0.23          |
| (1,1613) | 1:B:136:SER:H    | 1:B:135:SER:H   | 2        | 0.23          |
| (1,1609) | 1:B:135:SER:HA   | 1:B:145:VAL:HA  | 4        | 0.23          |
| (1,1607) | 1:B:135:SER:HA   | 1:B:145:VAL:HA  | 4        | 0.23          |
| (1,1542) | 1:B:128:VAL:H    | 1:B:126:ALA:H   | 4        | 0.23          |
| (1,1476) | 1:B:123:ARG:HA   | 1:B:123:ARG:HD2 | 4        | 0.23          |
| (1,1476) | 1:B:123:ARG:HA   | 1:B:123:ARG:HD3 | 4        | 0.23          |
| (1,1460) | 1:B:122:TYR:HB2  | 1:B:122:TYR:HA  | 8        | 0.23          |
| (1,1460) | 1:B:122:TYR:HB3  | 1:B:122:TYR:HA  | 8        | 0.23          |
| (1,1458) | 1:B:122:TYR:HB2  | 1:B:122:TYR:HA  | 8        | 0.23          |
| (1,1458) | 1:B:122:TYR:HB3  | 1:B:122:TYR:HA  | 8        | 0.23          |
| (1,1457) | 1:B:122:TYR:HA   | 1:B:98:ILE:H    | 8        | 0.23          |
| (1,1450) | 1:B:121:LYS:HA   | 1:B:99:GLU:HA   | 8        | 0.23          |
| (1,1413) | 1:B:117:GLU:HA   | 1:B:117:GLU:H   | 4        | 0.23          |
| (1,1321) | 1:B:110:GLU:H    | 1:B:110:GLU:HA  | 5        | 0.23          |
| (1,1287) | 1:B:106:GLU:HB2  | 1:B:106:GLU:H   | 2        | 0.23          |
| (1,1287) | 1:B:106:GLU:HB3  | 1:B:106:GLU:H   | 2        | 0.23          |
| (1,1281) | 1:B:105:GLU:HG2  | 1:B:105:GLU:H   | 9        | 0.23          |
| (1,1281) | 1:B:105:GLU:HG3  | 1:B:105:GLU:H   | 9        | 0.23          |
| (1,1280) | 1:B:105:GLU:HG2  | 1:B:105:GLU:H   | 9        | 0.23          |
| (1,1280) | 1:B:105:GLU:HG3  | 1:B:105:GLU:H   | 9        | 0.23          |
| (1,1266) | 1:B:103:LYS:HA   | 1:B:118:PHE:H   | 1        | 0.23          |
| (1,1245) | 1:B:101:HIS:HB3  | 1:B:101:HIS:H   | 7        | 0.23          |
| (1,1239) | 1:B:101:HIS:HA   | 1:B:101:HIS:HD2 | 9        | 0.23          |
| (1,1227) | 1:B:100:VAL:HA   | 1:B:100:VAL:H   | 1        | 0.23          |
| (1,1227) | 1:B:100:VAL:HA   | 1:B:100:VAL:H   | 9        | 0.23          |
| (1,1206) | 1:B:98:ILE:HB    | 1:B:98:ILE:H    | 3        | 0.23          |
| (1,1206) | 1:B:98:ILE:HB    | 1:B:98:ILE:H    | 5        | 0.23          |
| (1,120)  | 1:A:78:ASN:HA    | 1:A:78:ASN:HB3  | 6        | 0.23          |
| (1,1197) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 9        | 0.23          |
| (1,1196) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 9        | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1172) | 1:B:95:GLY:HA2  | 1:B:96:ASP:H    | 2        | 0.23          |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD11 | 1        | 0.23          |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD12 | 1        | 0.23          |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD13 | 1        | 0.23          |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD21 | 1        | 0.23          |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD22 | 1        | 0.23          |
| (1,1166) | 1:B:95:GLY:HA3  | 1:B:94:LEU:HD23 | 1        | 0.23          |
| (1,1148) | 1:B:92:LYS:H    | 1:B:101:HIS:H   | 1        | 0.23          |
| (1,1145) | 1:B:92:LYS:H    | 1:B:93:VAL:H    | 7        | 0.23          |
| (1,1139) | 1:B:92:LYS:H    | 1:B:91:VAL:HA   | 3        | 0.23          |
| (1,1139) | 1:B:92:LYS:H    | 1:B:91:VAL:HA   | 9        | 0.23          |
| (1,1119) | 1:B:89:LEU:H    | 1:B:90:LYS:H    | 8        | 0.23          |
| (1,108)  | 1:A:77:VAL:HG11 | 1:A:79:LEU:H    | 9        | 0.23          |
| (1,108)  | 1:A:77:VAL:HG12 | 1:A:79:LEU:H    | 9        | 0.23          |
| (1,108)  | 1:A:77:VAL:HG13 | 1:A:79:LEU:H    | 9        | 0.23          |
| (1,1056) | 1:B:84:PHE:H    | 1:B:81:VAL:HB   | 7        | 0.23          |
| (1,105)  | 1:A:77:VAL:HG21 | 1:A:79:LEU:HG   | 4        | 0.23          |
| (1,105)  | 1:A:77:VAL:HG22 | 1:A:79:LEU:HG   | 4        | 0.23          |
| (1,105)  | 1:A:77:VAL:HG23 | 1:A:79:LEU:HG   | 4        | 0.23          |
| (1,1042) | 1:B:83:HIS:HA   | 1:B:83:HIS:HB3  | 1        | 0.23          |
| (1,1041) | 1:B:83:HIS:HA   | 1:B:83:HIS:HB3  | 1        | 0.23          |
| (1,1035) | 1:B:81:VAL:HG21 | 1:B:143:LEU:HA  | 2        | 0.23          |
| (1,1035) | 1:B:81:VAL:HG22 | 1:B:143:LEU:HA  | 2        | 0.23          |
| (1,1035) | 1:B:81:VAL:HG23 | 1:B:143:LEU:HA  | 2        | 0.23          |
| (1,102)  | 1:A:77:VAL:HG11 | 1:A:78:ASN:H    | 7        | 0.23          |
| (1,102)  | 1:A:77:VAL:HG12 | 1:A:78:ASN:H    | 7        | 0.23          |
| (1,102)  | 1:A:77:VAL:HG13 | 1:A:78:ASN:H    | 7        | 0.23          |
| (1,987)  | 1:B:78:ASN:HA   | 1:B:78:ASN:HB3  | 1        | 0.22          |
| (1,969)  | 1:B:77:VAL:HG11 | 1:B:78:ASN:H    | 7        | 0.22          |
| (1,969)  | 1:B:77:VAL:HG12 | 1:B:78:ASN:H    | 7        | 0.22          |
| (1,969)  | 1:B:77:VAL:HG13 | 1:B:78:ASN:H    | 7        | 0.22          |
| (1,940)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2 | 4        | 0.22          |
| (1,937)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2 | 4        | 0.22          |
| (1,934)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2 | 4        | 0.22          |
| (1,930)  | 1:B:76:SER:HB2  | 1:B:77:VAL:H    | 1        | 0.22          |
| (1,915)  | 1:B:75:PHE:HA   | 1:B:75:PHE:HB3  | 4        | 0.22          |
| (1,881)  | 1:B:68:MET:HE1  | 1:B:122:TYR:HD1 | 4        | 0.22          |
| (1,881)  | 1:B:68:MET:HE1  | 1:B:122:TYR:HD2 | 4        | 0.22          |
| (1,881)  | 1:B:68:MET:HE2  | 1:B:122:TYR:HD1 | 4        | 0.22          |
| (1,881)  | 1:B:68:MET:HE2  | 1:B:122:TYR:HD2 | 4        | 0.22          |
| (1,881)  | 1:B:68:MET:HE3  | 1:B:122:TYR:HD1 | 4        | 0.22          |
| (1,881)  | 1:B:68:MET:HE3  | 1:B:122:TYR:HD2 | 4        | 0.22          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,847) | 1:A:147:GLY:HA2  | 1:A:147:GLY:H    | 2        | 0.22          |
| (1,835) | 1:A:146:ASP:HB2  | 1:A:146:ASP:HA   | 6        | 0.22          |
| (1,832) | 1:A:146:ASP:HB2  | 1:A:146:ASP:HA   | 6        | 0.22          |
| (1,822) | 1:A:145:VAL:HA   | 1:A:146:ASP:H    | 3        | 0.22          |
| (1,822) | 1:A:145:VAL:HA   | 1:A:146:ASP:H    | 8        | 0.22          |
| (1,822) | 1:A:145:VAL:HA   | 1:A:146:ASP:H    | 9        | 0.22          |
| (1,816) | 1:A:145:VAL:HA   | 1:A:145:VAL:H    | 2        | 0.22          |
| (1,816) | 1:A:145:VAL:HA   | 1:A:145:VAL:H    | 6        | 0.22          |
| (1,770) | 1:A:141:GLY:H    | 1:A:140:ASP:H    | 1        | 0.22          |
| (1,768) | 1:A:141:GLY:H    | 1:A:140:ASP:H    | 1        | 0.22          |
| (1,746) | 1:A:136:SER:H    | 1:A:135:SER:H    | 3        | 0.22          |
| (1,745) | 1:A:136:SER:H    | 1:A:135:SER:H    | 4        | 0.22          |
| (1,73)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2  | 4        | 0.22          |
| (1,717) | 1:A:133:ILE:HG21 | 1:A:132:THR:H    | 6        | 0.22          |
| (1,717) | 1:A:133:ILE:HG22 | 1:A:132:THR:H    | 6        | 0.22          |
| (1,717) | 1:A:133:ILE:HG23 | 1:A:132:THR:H    | 6        | 0.22          |
| (1,70)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2  | 4        | 0.22          |
| (1,682) | 1:A:129:ASP:H    | 1:A:128:VAL:HA   | 4        | 0.22          |
| (1,67)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2  | 4        | 0.22          |
| (1,656) | 1:A:125:PRO:HA   | 1:A:127:ASP:H    | 4        | 0.22          |
| (1,63)  | 1:A:76:SER:HB2   | 1:A:77:VAL:H     | 1        | 0.22          |
| (1,609) | 1:A:123:ARG:HA   | 1:A:123:ARG:HD2  | 4        | 0.22          |
| (1,609) | 1:A:123:ARG:HA   | 1:A:123:ARG:HD3  | 4        | 0.22          |
| (1,593) | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA   | 6        | 0.22          |
| (1,593) | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA   | 6        | 0.22          |
| (1,591) | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA   | 6        | 0.22          |
| (1,591) | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA   | 6        | 0.22          |
| (1,580) | 1:A:120:ARG:H    | 1:A:100:VAL:H    | 9        | 0.22          |
| (1,546) | 1:A:117:GLU:HA   | 1:A:117:GLU:H    | 2        | 0.22          |
| (1,48)  | 1:A:75:PHE:HA    | 1:A:75:PHE:HB3   | 4        | 0.22          |
| (1,473) | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG21 | 1        | 0.22          |
| (1,473) | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG22 | 1        | 0.22          |
| (1,473) | 1:A:111:HIS:HB3  | 1:A:114:ILE:HG23 | 1        | 0.22          |
| (1,447) | 1:A:109:ASP:H    | 1:A:109:ASP:HB2  | 4        | 0.22          |
| (1,447) | 1:A:109:ASP:H    | 1:A:109:ASP:HB3  | 4        | 0.22          |
| (1,411) | 1:A:105:GLU:HB2  | 1:A:105:GLU:H    | 4        | 0.22          |
| (1,411) | 1:A:105:GLU:HB3  | 1:A:105:GLU:H    | 4        | 0.22          |
| (1,369) | 1:A:101:HIS:H    | 1:A:100:VAL:HA   | 8        | 0.22          |
| (1,360) | 1:A:100:VAL:HA   | 1:A:100:VAL:H    | 6        | 0.22          |
| (1,305) | 1:A:95:GLY:HA2   | 1:A:96:ASP:H     | 8        | 0.22          |
| (1,292) | 1:A:94:LEU:HD11  | 1:A:95:GLY:H     | 1        | 0.22          |
| (1,292) | 1:A:94:LEU:HD12  | 1:A:95:GLY:H     | 1        | 0.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,292)  | 1:A:94:LEU:HD13  | 1:A:95:GLY:H    | 1        | 0.22          |
| (1,292)  | 1:A:94:LEU:HD21  | 1:A:95:GLY:H    | 1        | 0.22          |
| (1,292)  | 1:A:94:LEU:HD22  | 1:A:95:GLY:H    | 1        | 0.22          |
| (1,292)  | 1:A:94:LEU:HD23  | 1:A:95:GLY:H    | 1        | 0.22          |
| (1,276)  | 1:A:92:LYS:H     | 1:A:92:LYS:HA   | 8        | 0.22          |
| (1,272)  | 1:A:92:LYS:H     | 1:A:91:VAL:HA   | 4        | 0.22          |
| (1,272)  | 1:A:92:LYS:H     | 1:A:91:VAL:HA   | 5        | 0.22          |
| (1,250)  | 1:A:89:LEU:HD21  | 1:A:89:LEU:H    | 2        | 0.22          |
| (1,250)  | 1:A:89:LEU:HD22  | 1:A:89:LEU:H    | 2        | 0.22          |
| (1,250)  | 1:A:89:LEU:HD23  | 1:A:89:LEU:H    | 2        | 0.22          |
| (1,239)  | 1:A:89:LEU:H     | 1:A:87:GLU:HA   | 9        | 0.22          |
| (1,228)  | 1:A:87:GLU:H     | 1:A:88:GLU:H    | 6        | 0.22          |
| (1,225)  | 1:A:87:GLU:H     | 1:A:88:GLU:H    | 6        | 0.22          |
| (1,199)  | 1:A:84:PHE:HB2   | 1:A:85:SER:H    | 2        | 0.22          |
| (1,199)  | 1:A:84:PHE:HB3   | 1:A:85:SER:H    | 2        | 0.22          |
| (1,175)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB3  | 9        | 0.22          |
| (1,1749) | 1:A:115:SER:HB3  | 1:B:119:HIS:HE1 | 8        | 0.22          |
| (1,1744) | 1:A:114:ILE:HA   | 1:B:120:ARG:HB2 | 6        | 0.22          |
| (1,1744) | 1:A:114:ILE:HA   | 1:B:120:ARG:HB3 | 6        | 0.22          |
| (1,174)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB3  | 9        | 0.22          |
| (1,1714) | 1:B:147:GLY:HA2  | 1:B:147:GLY:H   | 2        | 0.22          |
| (1,1702) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 6        | 0.22          |
| (1,1699) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 6        | 0.22          |
| (1,1689) | 1:B:145:VAL:HA   | 1:B:146:ASP:H   | 3        | 0.22          |
| (1,1689) | 1:B:145:VAL:HA   | 1:B:146:ASP:H   | 8        | 0.22          |
| (1,1683) | 1:B:145:VAL:HA   | 1:B:145:VAL:H   | 2        | 0.22          |
| (1,1672) | 1:B:144:THR:HG21 | 1:B:145:VAL:H   | 4        | 0.22          |
| (1,1672) | 1:B:144:THR:HG22 | 1:B:145:VAL:H   | 4        | 0.22          |
| (1,1672) | 1:B:144:THR:HG23 | 1:B:145:VAL:H   | 4        | 0.22          |
| (1,1650) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1650) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1650) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1650) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1650) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1650) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1649) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1649) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1649) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1649) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1649) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1649) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H   | 2        | 0.22          |
| (1,1613) | 1:B:136:SER:H    | 1:B:135:SER:H   | 3        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1612) | 1:B:136:SER:H    | 1:B:135:SER:H    | 4        | 0.22          |
| (1,1584) | 1:B:133:ILE:HG21 | 1:B:132:THR:H    | 6        | 0.22          |
| (1,1584) | 1:B:133:ILE:HG22 | 1:B:132:THR:H    | 6        | 0.22          |
| (1,1584) | 1:B:133:ILE:HG23 | 1:B:132:THR:H    | 6        | 0.22          |
| (1,1549) | 1:B:129:ASP:H    | 1:B:128:VAL:HA   | 4        | 0.22          |
| (1,1523) | 1:B:125:PRO:HA   | 1:B:127:ASP:H    | 4        | 0.22          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD11 | 8        | 0.22          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD12 | 8        | 0.22          |
| (1,1514) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HD13 | 8        | 0.22          |
| (1,1447) | 1:B:120:ARG:H    | 1:B:100:VAL:H    | 9        | 0.22          |
| (1,1413) | 1:B:117:GLU:HA   | 1:B:117:GLU:H    | 2        | 0.22          |
| (1,14)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HD1  | 4        | 0.22          |
| (1,14)   | 1:A:68:MET:HE1   | 1:A:122:TYR:HD2  | 4        | 0.22          |
| (1,14)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HD1  | 4        | 0.22          |
| (1,14)   | 1:A:68:MET:HE2   | 1:A:122:TYR:HD2  | 4        | 0.22          |
| (1,14)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HD1  | 4        | 0.22          |
| (1,14)   | 1:A:68:MET:HE3   | 1:A:122:TYR:HD2  | 4        | 0.22          |
| (1,138)  | 1:A:79:LEU:HD11  | 1:A:79:LEU:HA    | 7        | 0.22          |
| (1,138)  | 1:A:79:LEU:HD12  | 1:A:79:LEU:HA    | 7        | 0.22          |
| (1,138)  | 1:A:79:LEU:HD13  | 1:A:79:LEU:HA    | 7        | 0.22          |
| (1,138)  | 1:A:79:LEU:HD21  | 1:A:79:LEU:HA    | 7        | 0.22          |
| (1,138)  | 1:A:79:LEU:HD22  | 1:A:79:LEU:HA    | 7        | 0.22          |
| (1,138)  | 1:A:79:LEU:HD23  | 1:A:79:LEU:HA    | 7        | 0.22          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG21 | 1        | 0.22          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG22 | 1        | 0.22          |
| (1,1340) | 1:B:111:HIS:HB3  | 1:B:114:ILE:HG23 | 1        | 0.22          |
| (1,1314) | 1:B:109:ASP:H    | 1:B:109:ASP:HB2  | 4        | 0.22          |
| (1,1314) | 1:B:109:ASP:H    | 1:B:109:ASP:HB3  | 4        | 0.22          |
| (1,1278) | 1:B:105:GLU:HB2  | 1:B:105:GLU:H    | 4        | 0.22          |
| (1,1278) | 1:B:105:GLU:HB3  | 1:B:105:GLU:H    | 4        | 0.22          |
| (1,1236) | 1:B:101:HIS:H    | 1:B:100:VAL:HA   | 8        | 0.22          |
| (1,1227) | 1:B:100:VAL:HA   | 1:B:100:VAL:H    | 6        | 0.22          |
| (1,120)  | 1:A:78:ASN:HA    | 1:A:78:ASN:HB3   | 1        | 0.22          |
| (1,1172) | 1:B:95:GLY:HA2   | 1:B:96:ASP:H     | 8        | 0.22          |
| (1,1159) | 1:B:94:LEU:HD11  | 1:B:95:GLY:H     | 1        | 0.22          |
| (1,1159) | 1:B:94:LEU:HD12  | 1:B:95:GLY:H     | 1        | 0.22          |
| (1,1159) | 1:B:94:LEU:HD13  | 1:B:95:GLY:H     | 1        | 0.22          |
| (1,1159) | 1:B:94:LEU:HD21  | 1:B:95:GLY:H     | 1        | 0.22          |
| (1,1159) | 1:B:94:LEU:HD22  | 1:B:95:GLY:H     | 1        | 0.22          |
| (1,1159) | 1:B:94:LEU:HD23  | 1:B:95:GLY:H     | 1        | 0.22          |
| (1,1146) | 1:B:92:LYS:H     | 1:B:99:GLU:H     | 2        | 0.22          |
| (1,1143) | 1:B:92:LYS:H     | 1:B:92:LYS:HA    | 8        | 0.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1139) | 1:B:92:LYS:H     | 1:B:91:VAL:HA   | 5        | 0.22          |
| (1,1120) | 1:B:89:LEU:HA    | 1:B:90:LYS:H    | 5        | 0.22          |
| (1,1117) | 1:B:89:LEU:HD21  | 1:B:89:LEU:H    | 2        | 0.22          |
| (1,1117) | 1:B:89:LEU:HD22  | 1:B:89:LEU:H    | 2        | 0.22          |
| (1,1117) | 1:B:89:LEU:HD23  | 1:B:89:LEU:H    | 2        | 0.22          |
| (1,1106) | 1:B:89:LEU:H     | 1:B:87:GLU:HA   | 9        | 0.22          |
| (1,1095) | 1:B:87:GLU:H     | 1:B:88:GLU:H    | 6        | 0.22          |
| (1,1092) | 1:B:87:GLU:H     | 1:B:88:GLU:H    | 6        | 0.22          |
| (1,1066) | 1:B:84:PHE:HB2   | 1:B:85:SER:H    | 2        | 0.22          |
| (1,1066) | 1:B:84:PHE:HB3   | 1:B:85:SER:H    | 2        | 0.22          |
| (1,1042) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3  | 9        | 0.22          |
| (1,1041) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3  | 9        | 0.22          |
| (1,1005) | 1:B:79:LEU:HD11  | 1:B:79:LEU:HA   | 7        | 0.22          |
| (1,1005) | 1:B:79:LEU:HD12  | 1:B:79:LEU:HA   | 7        | 0.22          |
| (1,1005) | 1:B:79:LEU:HD13  | 1:B:79:LEU:HA   | 7        | 0.22          |
| (1,1005) | 1:B:79:LEU:HD21  | 1:B:79:LEU:HA   | 7        | 0.22          |
| (1,1005) | 1:B:79:LEU:HD22  | 1:B:79:LEU:HA   | 7        | 0.22          |
| (1,1005) | 1:B:79:LEU:HD23  | 1:B:79:LEU:HA   | 7        | 0.22          |
| (1,997)  | 1:B:78:ASN:HB2   | 1:B:79:LEU:H    | 2        | 0.21          |
| (1,952)  | 1:B:77:VAL:HB    | 1:B:75:PHE:HD1  | 7        | 0.21          |
| (1,952)  | 1:B:77:VAL:HB    | 1:B:75:PHE:HD2  | 7        | 0.21          |
| (1,945)  | 1:B:76:SER:HA    | 1:B:146:ASP:HA  | 9        | 0.21          |
| (1,941)  | 1:B:76:SER:HA    | 1:B:146:ASP:HA  | 9        | 0.21          |
| (1,940)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2 | 6        | 0.21          |
| (1,937)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2 | 6        | 0.21          |
| (1,934)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB2 | 6        | 0.21          |
| (1,905)  | 1:B:74:ARG:H     | 1:B:73:ASP:H    | 8        | 0.21          |
| (1,904)  | 1:B:74:ARG:H     | 1:B:73:ASP:H    | 8        | 0.21          |
| (1,898)  | 1:B:73:ASP:H     | 1:B:72:LYS:HB2  | 5        | 0.21          |
| (1,898)  | 1:B:73:ASP:H     | 1:B:72:LYS:HB3  | 5        | 0.21          |
| (1,875)  | 1:B:68:MET:HG2   | 1:B:68:MET:H    | 3        | 0.21          |
| (1,875)  | 1:B:68:MET:HG3   | 1:B:68:MET:H    | 3        | 0.21          |
| (1,866)  | 1:A:152:VAL:H    | 1:A:151:GLN:H   | 3        | 0.21          |
| (1,85)   | 1:A:77:VAL:HB    | 1:A:75:PHE:HD1  | 7        | 0.21          |
| (1,85)   | 1:A:77:VAL:HB    | 1:A:75:PHE:HD2  | 7        | 0.21          |
| (1,822)  | 1:A:145:VAL:HA   | 1:A:146:ASP:H   | 4        | 0.21          |
| (1,822)  | 1:A:145:VAL:HA   | 1:A:146:ASP:H   | 7        | 0.21          |
| (1,817)  | 1:A:145:VAL:HB   | 1:A:145:VAL:H   | 8        | 0.21          |
| (1,816)  | 1:A:145:VAL:HA   | 1:A:145:VAL:H   | 5        | 0.21          |
| (1,805)  | 1:A:144:THR:HG21 | 1:A:145:VAL:H   | 4        | 0.21          |
| (1,805)  | 1:A:144:THR:HG22 | 1:A:145:VAL:H   | 4        | 0.21          |
| (1,805)  | 1:A:144:THR:HG23 | 1:A:145:VAL:H   | 4        | 0.21          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,8)   | 1:A:68:MET:HG2   | 1:A:68:MET:H    | 3        | 0.21          |
| (1,8)   | 1:A:68:MET:HG3   | 1:A:68:MET:H    | 3        | 0.21          |
| (1,78)  | 1:A:76:SER:HA    | 1:A:146:ASP:HA  | 9        | 0.21          |
| (1,770) | 1:A:141:GLY:H    | 1:A:140:ASP:H   | 6        | 0.21          |
| (1,770) | 1:A:141:GLY:H    | 1:A:140:ASP:H   | 8        | 0.21          |
| (1,768) | 1:A:141:GLY:H    | 1:A:140:ASP:H   | 6        | 0.21          |
| (1,768) | 1:A:141:GLY:H    | 1:A:140:ASP:H   | 8        | 0.21          |
| (1,752) | 1:A:137:LEU:H    | 1:A:137:LEU:HB2 | 9        | 0.21          |
| (1,752) | 1:A:137:LEU:H    | 1:A:137:LEU:HB3 | 9        | 0.21          |
| (1,74)  | 1:A:76:SER:HA    | 1:A:146:ASP:HA  | 9        | 0.21          |
| (1,731) | 1:A:134:THR:HG21 | 1:A:135:SER:H   | 5        | 0.21          |
| (1,731) | 1:A:134:THR:HG22 | 1:A:135:SER:H   | 5        | 0.21          |
| (1,731) | 1:A:134:THR:HG23 | 1:A:135:SER:H   | 5        | 0.21          |
| (1,73)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2 | 6        | 0.21          |
| (1,70)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2 | 6        | 0.21          |
| (1,680) | 1:A:128:VAL:H    | 1:A:129:ASP:H   | 2        | 0.21          |
| (1,670) | 1:A:127:ASP:HB3  | 1:A:127:ASP:H   | 2        | 0.21          |
| (1,67)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2 | 6        | 0.21          |
| (1,650) | 1:A:125:PRO:HD3  | 1:A:124:ILE:HB  | 8        | 0.21          |
| (1,573) | 1:A:119:HIS:HA   | 1:A:119:HIS:HD2 | 8        | 0.21          |
| (1,569) | 1:A:119:HIS:HA   | 1:A:101:HIS:HA  | 2        | 0.21          |
| (1,564) | 1:A:118:PHE:HD1  | 1:A:118:PHE:H   | 3        | 0.21          |
| (1,564) | 1:A:118:PHE:HD2  | 1:A:118:PHE:H   | 3        | 0.21          |
| (1,564) | 1:A:118:PHE:HD1  | 1:A:118:PHE:H   | 9        | 0.21          |
| (1,564) | 1:A:118:PHE:HD2  | 1:A:118:PHE:H   | 9        | 0.21          |
| (1,469) | 1:A:111:HIS:HB2  | 1:A:112:GLY:H   | 4        | 0.21          |
| (1,469) | 1:A:111:HIS:HB2  | 1:A:112:GLY:H   | 5        | 0.21          |
| (1,469) | 1:A:111:HIS:HB2  | 1:A:112:GLY:H   | 7        | 0.21          |
| (1,459) | 1:A:111:HIS:H    | 1:A:110:GLU:H   | 4        | 0.21          |
| (1,458) | 1:A:111:HIS:H    | 1:A:110:GLU:H   | 4        | 0.21          |
| (1,411) | 1:A:105:GLU:HB2  | 1:A:105:GLU:H   | 1        | 0.21          |
| (1,411) | 1:A:105:GLU:HB3  | 1:A:105:GLU:H   | 1        | 0.21          |
| (1,398) | 1:A:103:LYS:HD2  | 1:A:118:PHE:H   | 4        | 0.21          |
| (1,398) | 1:A:103:LYS:HD3  | 1:A:118:PHE:H   | 4        | 0.21          |
| (1,38)  | 1:A:74:ARG:H     | 1:A:73:ASP:H    | 8        | 0.21          |
| (1,379) | 1:A:101:HIS:HB2  | 1:A:101:HIS:H   | 7        | 0.21          |
| (1,37)  | 1:A:74:ARG:H     | 1:A:73:ASP:H    | 8        | 0.21          |
| (1,368) | 1:A:101:HIS:HB2  | 1:A:92:LYS:HB2  | 1        | 0.21          |
| (1,368) | 1:A:101:HIS:HB2  | 1:A:92:LYS:HB3  | 1        | 0.21          |
| (1,360) | 1:A:100:VAL:HA   | 1:A:100:VAL:H   | 3        | 0.21          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG11 | 2        | 0.21          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG12 | 2        | 0.21          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG13 | 2        | 0.21          |
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG21 | 2        | 0.21          |
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG22 | 2        | 0.21          |
| (1,327)  | 1:A:97:VAL:HA    | 1:A:97:VAL:HG23 | 2        | 0.21          |
| (1,31)   | 1:A:73:ASP:H     | 1:A:72:LYS:HB2  | 5        | 0.21          |
| (1,31)   | 1:A:73:ASP:H     | 1:A:72:LYS:HB3  | 5        | 0.21          |
| (1,301)  | 1:A:95:GLY:H     | 1:A:94:LEU:HG   | 6        | 0.21          |
| (1,293)  | 1:A:94:LEU:H     | 1:A:95:GLY:H    | 9        | 0.21          |
| (1,289)  | 1:A:94:LEU:H     | 1:A:93:VAL:HB   | 5        | 0.21          |
| (1,279)  | 1:A:92:LYS:H     | 1:A:99:GLU:H    | 2        | 0.21          |
| (1,253)  | 1:A:89:LEU:HA    | 1:A:90:LYS:H    | 5        | 0.21          |
| (1,252)  | 1:A:89:LEU:H     | 1:A:90:LYS:H    | 2        | 0.21          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG2  | 2        | 0.21          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG3  | 2        | 0.21          |
| (1,237)  | 1:A:89:LEU:H     | 1:A:85:SER:H    | 4        | 0.21          |
| (1,215)  | 1:A:85:SER:HB3   | 1:A:89:LEU:H    | 5        | 0.21          |
| (1,203)  | 1:A:84:PHE:HE1   | 1:A:116:ARG:H   | 9        | 0.21          |
| (1,203)  | 1:A:84:PHE:HE2   | 1:A:116:ARG:H   | 9        | 0.21          |
| (1,1733) | 1:B:152:VAL:H    | 1:B:151:GLN:H   | 3        | 0.21          |
| (1,1689) | 1:B:145:VAL:HA   | 1:B:146:ASP:H   | 4        | 0.21          |
| (1,1689) | 1:B:145:VAL:HA   | 1:B:146:ASP:H   | 7        | 0.21          |
| (1,1689) | 1:B:145:VAL:HA   | 1:B:146:ASP:H   | 9        | 0.21          |
| (1,1684) | 1:B:145:VAL:HB   | 1:B:145:VAL:H   | 8        | 0.21          |
| (1,1683) | 1:B:145:VAL:HA   | 1:B:145:VAL:H   | 6        | 0.21          |
| (1,1637) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 6        | 0.21          |
| (1,1637) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 8        | 0.21          |
| (1,1635) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 6        | 0.21          |
| (1,1635) | 1:B:141:GLY:H    | 1:B:140:ASP:H   | 8        | 0.21          |
| (1,1620) | 1:B:137:LEU:H    | 1:B:137:LEU:HG  | 3        | 0.21          |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB2 | 9        | 0.21          |
| (1,1619) | 1:B:137:LEU:H    | 1:B:137:LEU:HB3 | 9        | 0.21          |
| (1,1598) | 1:B:134:THR:HG21 | 1:B:135:SER:H   | 5        | 0.21          |
| (1,1598) | 1:B:134:THR:HG22 | 1:B:135:SER:H   | 5        | 0.21          |
| (1,1598) | 1:B:134:THR:HG23 | 1:B:135:SER:H   | 5        | 0.21          |
| (1,1572) | 1:B:132:THR:HG1  | 1:B:133:ILE:H   | 9        | 0.21          |
| (1,1547) | 1:B:128:VAL:H    | 1:B:129:ASP:H   | 2        | 0.21          |
| (1,1537) | 1:B:127:ASP:HB3  | 1:B:127:ASP:H   | 2        | 0.21          |
| (1,1517) | 1:B:125:PRO:HD3  | 1:B:124:ILE:HB  | 8        | 0.21          |
| (1,1460) | 1:B:122:TYR:HB2  | 1:B:122:TYR:HA  | 6        | 0.21          |
| (1,1460) | 1:B:122:TYR:HB3  | 1:B:122:TYR:HA  | 6        | 0.21          |
| (1,1458) | 1:B:122:TYR:HB2  | 1:B:122:TYR:HA  | 6        | 0.21          |
| (1,1458) | 1:B:122:TYR:HB3  | 1:B:122:TYR:HA  | 6        | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1440) | 1:B:119:HIS:HA  | 1:B:119:HIS:HD2 | 8        | 0.21          |
| (1,1436) | 1:B:119:HIS:HA  | 1:B:101:HIS:HA  | 2        | 0.21          |
| (1,1431) | 1:B:118:PHE:HD1 | 1:B:118:PHE:H   | 3        | 0.21          |
| (1,1431) | 1:B:118:PHE:HD2 | 1:B:118:PHE:H   | 3        | 0.21          |
| (1,1431) | 1:B:118:PHE:HD1 | 1:B:118:PHE:H   | 9        | 0.21          |
| (1,1431) | 1:B:118:PHE:HD2 | 1:B:118:PHE:H   | 9        | 0.21          |
| (1,1336) | 1:B:111:HIS:HB2 | 1:B:112:GLY:H   | 4        | 0.21          |
| (1,1336) | 1:B:111:HIS:HB2 | 1:B:112:GLY:H   | 5        | 0.21          |
| (1,1336) | 1:B:111:HIS:HB2 | 1:B:112:GLY:H   | 7        | 0.21          |
| (1,1326) | 1:B:111:HIS:H   | 1:B:110:GLU:H   | 4        | 0.21          |
| (1,1325) | 1:B:111:HIS:H   | 1:B:110:GLU:H   | 4        | 0.21          |
| (1,130)  | 1:A:78:ASN:HB2  | 1:A:79:LEU:H    | 2        | 0.21          |
| (1,1265) | 1:B:103:LYS:HD2 | 1:B:118:PHE:H   | 4        | 0.21          |
| (1,1265) | 1:B:103:LYS:HD3 | 1:B:118:PHE:H   | 4        | 0.21          |
| (1,1246) | 1:B:101:HIS:HB2 | 1:B:101:HIS:H   | 7        | 0.21          |
| (1,1235) | 1:B:101:HIS:HB2 | 1:B:92:LYS:HB2  | 1        | 0.21          |
| (1,1235) | 1:B:101:HIS:HB2 | 1:B:92:LYS:HB3  | 1        | 0.21          |
| (1,1227) | 1:B:100:VAL:HA  | 1:B:100:VAL:H   | 3        | 0.21          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG11 | 2        | 0.21          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG12 | 2        | 0.21          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG13 | 2        | 0.21          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG21 | 2        | 0.21          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG22 | 2        | 0.21          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG23 | 2        | 0.21          |
| (1,1160) | 1:B:94:LEU:H    | 1:B:95:GLY:H    | 9        | 0.21          |
| (1,1156) | 1:B:94:LEU:H    | 1:B:93:VAL:HB   | 5        | 0.21          |
| (1,1139) | 1:B:92:LYS:H    | 1:B:91:VAL:HA   | 4        | 0.21          |
| (1,1119) | 1:B:89:LEU:H    | 1:B:90:LYS:H    | 2        | 0.21          |
| (1,1104) | 1:B:89:LEU:H    | 1:B:85:SER:H    | 4        | 0.21          |
| (1,1082) | 1:B:85:SER:HB3  | 1:B:89:LEU:H    | 5        | 0.21          |
| (1,1070) | 1:B:84:PHE:HE1  | 1:B:116:ARG:H   | 2        | 0.21          |
| (1,1070) | 1:B:84:PHE:HE2  | 1:B:116:ARG:H   | 2        | 0.21          |
| (1,1070) | 1:B:84:PHE:HE1  | 1:B:116:ARG:H   | 9        | 0.21          |
| (1,1070) | 1:B:84:PHE:HE2  | 1:B:116:ARG:H   | 9        | 0.21          |
| (1,1047) | 1:B:83:HIS:HB2  | 1:B:83:HIS:H    | 5        | 0.21          |
| (1,988)  | 1:B:78:ASN:HA   | 1:B:78:ASN:HB2  | 5        | 0.2           |
| (1,988)  | 1:B:78:ASN:HA   | 1:B:78:ASN:HB2  | 9        | 0.2           |
| (1,986)  | 1:B:77:VAL:HB   | 1:B:146:ASP:HB3 | 3        | 0.2           |
| (1,918)  | 1:B:75:PHE:HA   | 1:B:76:SER:H    | 8        | 0.2           |
| (1,9)    | 1:A:68:MET:HE1  | 1:A:68:MET:H    | 9        | 0.2           |
| (1,9)    | 1:A:68:MET:HE2  | 1:A:68:MET:H    | 9        | 0.2           |
| (1,9)    | 1:A:68:MET:HE3  | 1:A:68:MET:H    | 9        | 0.2           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,898) | 1:B:73:ASP:H     | 1:B:72:LYS:HB2   | 9        | 0.2           |
| (1,898) | 1:B:73:ASP:H     | 1:B:72:LYS:HB3   | 9        | 0.2           |
| (1,895) | 1:B:72:LYS:H     | 1:B:72:LYS:HA    | 4        | 0.2           |
| (1,892) | 1:B:71:GLU:H     | 1:B:71:GLU:HG2   | 2        | 0.2           |
| (1,892) | 1:B:71:GLU:H     | 1:B:71:GLU:HG3   | 2        | 0.2           |
| (1,883) | 1:B:70:LEU:H     | 1:B:70:LEU:HB2   | 2        | 0.2           |
| (1,822) | 1:A:145:VAL:HA   | 1:A:146:ASP:H    | 1        | 0.2           |
| (1,822) | 1:A:145:VAL:HA   | 1:A:146:ASP:H    | 2        | 0.2           |
| (1,816) | 1:A:145:VAL:HA   | 1:A:145:VAL:H    | 1        | 0.2           |
| (1,816) | 1:A:145:VAL:HA   | 1:A:145:VAL:H    | 4        | 0.2           |
| (1,816) | 1:A:145:VAL:HA   | 1:A:145:VAL:H    | 7        | 0.2           |
| (1,816) | 1:A:145:VAL:HA   | 1:A:145:VAL:H    | 9        | 0.2           |
| (1,794) | 1:A:144:THR:HG21 | 1:A:78:ASN:HA    | 4        | 0.2           |
| (1,794) | 1:A:144:THR:HG22 | 1:A:78:ASN:HA    | 4        | 0.2           |
| (1,794) | 1:A:144:THR:HG23 | 1:A:78:ASN:HA    | 4        | 0.2           |
| (1,78)  | 1:A:76:SER:HA    | 1:A:146:ASP:HA   | 7        | 0.2           |
| (1,77)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB3  | 5        | 0.2           |
| (1,755) | 1:A:138:SER:H    | 1:A:137:LEU:H    | 3        | 0.2           |
| (1,753) | 1:A:137:LEU:H    | 1:A:137:LEU:HG   | 3        | 0.2           |
| (1,746) | 1:A:136:SER:H    | 1:A:135:SER:H    | 5        | 0.2           |
| (1,746) | 1:A:136:SER:H    | 1:A:135:SER:H    | 6        | 0.2           |
| (1,74)  | 1:A:76:SER:HA    | 1:A:146:ASP:HA   | 7        | 0.2           |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG21 | 2        | 0.2           |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG22 | 2        | 0.2           |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG23 | 2        | 0.2           |
| (1,593) | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA   | 3        | 0.2           |
| (1,593) | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA   | 3        | 0.2           |
| (1,591) | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA   | 3        | 0.2           |
| (1,591) | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA   | 3        | 0.2           |
| (1,589) | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG21  | 2        | 0.2           |
| (1,589) | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG22  | 2        | 0.2           |
| (1,589) | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG23  | 2        | 0.2           |
| (1,589) | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG21  | 2        | 0.2           |
| (1,589) | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG22  | 2        | 0.2           |
| (1,589) | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG23  | 2        | 0.2           |
| (1,51)  | 1:A:75:PHE:HA    | 1:A:76:SER:H     | 8        | 0.2           |
| (1,478) | 1:A:112:GLY:HA2  | 1:A:112:GLY:H    | 4        | 0.2           |
| (1,464) | 1:A:111:HIS:H    | 1:A:111:HIS:HD2  | 8        | 0.2           |
| (1,457) | 1:A:111:HIS:H    | 1:A:109:ASP:HB2  | 7        | 0.2           |
| (1,457) | 1:A:111:HIS:H    | 1:A:109:ASP:HB3  | 7        | 0.2           |
| (1,427) | 1:A:107:ARG:HB3  | 1:A:107:ARG:H    | 6        | 0.2           |
| (1,411) | 1:A:105:GLU:HB2  | 1:A:105:GLU:H    | 5        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,411)  | 1:A:105:GLU:HB3 | 1:A:105:GLU:H   | 5        | 0.2           |
| (1,395)  | 1:A:103:LYS:HG2 | 1:A:103:LYS:H   | 6        | 0.2           |
| (1,395)  | 1:A:103:LYS:HG3 | 1:A:103:LYS:H   | 6        | 0.2           |
| (1,392)  | 1:A:102:GLY:H   | 1:A:118:PHE:H   | 7        | 0.2           |
| (1,379)  | 1:A:101:HIS:HB2 | 1:A:101:HIS:H   | 1        | 0.2           |
| (1,367)  | 1:A:101:HIS:HB3 | 1:A:92:LYS:HB2  | 6        | 0.2           |
| (1,367)  | 1:A:101:HIS:HB3 | 1:A:92:LYS:HB3  | 6        | 0.2           |
| (1,31)   | 1:A:73:ASP:H    | 1:A:72:LYS:HB2  | 9        | 0.2           |
| (1,31)   | 1:A:73:ASP:H    | 1:A:72:LYS:HB3  | 9        | 0.2           |
| (1,296)  | 1:A:94:LEU:H    | 1:A:99:GLU:H    | 5        | 0.2           |
| (1,291)  | 1:A:94:LEU:HD11 | 1:A:94:LEU:H    | 8        | 0.2           |
| (1,291)  | 1:A:94:LEU:HD12 | 1:A:94:LEU:H    | 8        | 0.2           |
| (1,291)  | 1:A:94:LEU:HD13 | 1:A:94:LEU:H    | 8        | 0.2           |
| (1,291)  | 1:A:94:LEU:HD21 | 1:A:94:LEU:H    | 8        | 0.2           |
| (1,291)  | 1:A:94:LEU:HD22 | 1:A:94:LEU:H    | 8        | 0.2           |
| (1,291)  | 1:A:94:LEU:HD23 | 1:A:94:LEU:H    | 8        | 0.2           |
| (1,280)  | 1:A:92:LYS:H    | 1:A:100:VAL:HA  | 2        | 0.2           |
| (1,28)   | 1:A:72:LYS:H    | 1:A:72:LYS:HA   | 4        | 0.2           |
| (1,278)  | 1:A:92:LYS:H    | 1:A:93:VAL:H    | 4        | 0.2           |
| (1,276)  | 1:A:92:LYS:H    | 1:A:92:LYS:HA   | 3        | 0.2           |
| (1,276)  | 1:A:92:LYS:H    | 1:A:92:LYS:HA   | 5        | 0.2           |
| (1,276)  | 1:A:92:LYS:H    | 1:A:92:LYS:HA   | 7        | 0.2           |
| (1,24)   | 1:A:71:GLU:H    | 1:A:69:ARG:HG2  | 7        | 0.2           |
| (1,24)   | 1:A:71:GLU:H    | 1:A:69:ARG:HG3  | 7        | 0.2           |
| (1,215)  | 1:A:85:SER:HB3  | 1:A:89:LEU:H    | 2        | 0.2           |
| (1,203)  | 1:A:84:PHE:HE1  | 1:A:116:ARG:H   | 2        | 0.2           |
| (1,203)  | 1:A:84:PHE:HE2  | 1:A:116:ARG:H   | 2        | 0.2           |
| (1,192)  | 1:A:84:PHE:HD1  | 1:A:83:HIS:HB3  | 5        | 0.2           |
| (1,192)  | 1:A:84:PHE:HD2  | 1:A:83:HIS:HB3  | 5        | 0.2           |
| (1,180)  | 1:A:83:HIS:HB2  | 1:A:83:HIS:H    | 5        | 0.2           |
| (1,176)  | 1:A:83:HIS:HB3  | 1:A:83:HIS:HD2  | 1        | 0.2           |
| (1,1689) | 1:B:145:VAL:HA  | 1:B:146:ASP:H   | 1        | 0.2           |
| (1,1683) | 1:B:145:VAL:HA  | 1:B:145:VAL:H   | 1        | 0.2           |
| (1,1683) | 1:B:145:VAL:HA  | 1:B:145:VAL:H   | 4        | 0.2           |
| (1,1683) | 1:B:145:VAL:HA  | 1:B:145:VAL:H   | 5        | 0.2           |
| (1,1683) | 1:B:145:VAL:HA  | 1:B:145:VAL:H   | 9        | 0.2           |
| (1,166)  | 1:A:81:VAL:HG11 | 1:A:118:PHE:HD1 | 9        | 0.2           |
| (1,166)  | 1:A:81:VAL:HG11 | 1:A:118:PHE:HD2 | 9        | 0.2           |
| (1,166)  | 1:A:81:VAL:HG12 | 1:A:118:PHE:HD1 | 9        | 0.2           |
| (1,166)  | 1:A:81:VAL:HG12 | 1:A:118:PHE:HD2 | 9        | 0.2           |
| (1,166)  | 1:A:81:VAL:HG13 | 1:A:118:PHE:HD1 | 9        | 0.2           |
| (1,166)  | 1:A:81:VAL:HG13 | 1:A:118:PHE:HD2 | 9        | 0.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,164)  | 1:A:81:VAL:HG21 | 1:A:84:PHE:H     | 4        | 0.2           |
| (1,164)  | 1:A:81:VAL:HG22 | 1:A:84:PHE:H     | 4        | 0.2           |
| (1,164)  | 1:A:81:VAL:HG23 | 1:A:84:PHE:H     | 4        | 0.2           |
| (1,1622) | 1:B:138:SER:H   | 1:B:137:LEU:H    | 3        | 0.2           |
| (1,1613) | 1:B:136:SER:H   | 1:B:135:SER:H    | 5        | 0.2           |
| (1,1613) | 1:B:136:SER:H   | 1:B:135:SER:H    | 6        | 0.2           |
| (1,161)  | 1:A:81:VAL:H    | 1:A:82:LYS:HA    | 4        | 0.2           |
| (1,1605) | 1:B:135:SER:HA  | 1:B:145:VAL:HG21 | 2        | 0.2           |
| (1,1605) | 1:B:135:SER:HA  | 1:B:145:VAL:HG22 | 2        | 0.2           |
| (1,1605) | 1:B:135:SER:HA  | 1:B:145:VAL:HG23 | 2        | 0.2           |
| (1,16)   | 1:A:70:LEU:H    | 1:A:70:LEU:HB2   | 2        | 0.2           |
| (1,1554) | 1:B:130:PRO:HG2 | 1:B:131:LEU:H    | 9        | 0.2           |
| (1,1554) | 1:B:130:PRO:HG3 | 1:B:131:LEU:H    | 9        | 0.2           |
| (1,1460) | 1:B:122:TYR:HB2 | 1:B:122:TYR:HA   | 3        | 0.2           |
| (1,1460) | 1:B:122:TYR:HB3 | 1:B:122:TYR:HA   | 3        | 0.2           |
| (1,1458) | 1:B:122:TYR:HB2 | 1:B:122:TYR:HA   | 3        | 0.2           |
| (1,1458) | 1:B:122:TYR:HB3 | 1:B:122:TYR:HA   | 3        | 0.2           |
| (1,1345) | 1:B:112:GLY:HA2 | 1:B:112:GLY:H    | 4        | 0.2           |
| (1,1331) | 1:B:111:HIS:H   | 1:B:111:HIS:HD2  | 6        | 0.2           |
| (1,1324) | 1:B:111:HIS:H   | 1:B:109:ASP:HB2  | 7        | 0.2           |
| (1,1324) | 1:B:111:HIS:H   | 1:B:109:ASP:HB3  | 7        | 0.2           |
| (1,1294) | 1:B:107:ARG:HB3 | 1:B:107:ARG:H    | 6        | 0.2           |
| (1,1282) | 1:B:105:GLU:HA  | 1:B:106:GLU:H    | 7        | 0.2           |
| (1,1278) | 1:B:105:GLU:HB2 | 1:B:105:GLU:H    | 1        | 0.2           |
| (1,1278) | 1:B:105:GLU:HB3 | 1:B:105:GLU:H    | 1        | 0.2           |
| (1,1278) | 1:B:105:GLU:HB2 | 1:B:105:GLU:H    | 5        | 0.2           |
| (1,1278) | 1:B:105:GLU:HB3 | 1:B:105:GLU:H    | 5        | 0.2           |
| (1,1262) | 1:B:103:LYS:HG2 | 1:B:103:LYS:H    | 6        | 0.2           |
| (1,1262) | 1:B:103:LYS:HG3 | 1:B:103:LYS:H    | 6        | 0.2           |
| (1,1259) | 1:B:102:GLY:H   | 1:B:118:PHE:H    | 7        | 0.2           |
| (1,1246) | 1:B:101:HIS:HB2 | 1:B:101:HIS:H    | 1        | 0.2           |
| (1,1234) | 1:B:101:HIS:HB3 | 1:B:92:LYS:HB2   | 6        | 0.2           |
| (1,1234) | 1:B:101:HIS:HB3 | 1:B:92:LYS:HB3   | 6        | 0.2           |
| (1,121)  | 1:A:78:ASN:HA   | 1:A:78:ASN:HB2   | 9        | 0.2           |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG11  | 3        | 0.2           |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG12  | 3        | 0.2           |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG13  | 3        | 0.2           |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG21  | 3        | 0.2           |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG22  | 3        | 0.2           |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG23  | 3        | 0.2           |
| (1,119)  | 1:A:77:VAL:HB   | 1:A:146:ASP:HB3  | 3        | 0.2           |
| (1,1168) | 1:B:95:GLY:H    | 1:B:94:LEU:HG    | 6        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1163) | 1:B:94:LEU:H    | 1:B:99:GLU:H    | 5        | 0.2           |
| (1,1158) | 1:B:94:LEU:HD11 | 1:B:94:LEU:H    | 8        | 0.2           |
| (1,1158) | 1:B:94:LEU:HD12 | 1:B:94:LEU:H    | 8        | 0.2           |
| (1,1158) | 1:B:94:LEU:HD13 | 1:B:94:LEU:H    | 8        | 0.2           |
| (1,1158) | 1:B:94:LEU:HD21 | 1:B:94:LEU:H    | 8        | 0.2           |
| (1,1158) | 1:B:94:LEU:HD22 | 1:B:94:LEU:H    | 8        | 0.2           |
| (1,1158) | 1:B:94:LEU:HD23 | 1:B:94:LEU:H    | 8        | 0.2           |
| (1,1147) | 1:B:92:LYS:H    | 1:B:100:VAL:HA  | 2        | 0.2           |
| (1,1145) | 1:B:92:LYS:H    | 1:B:93:VAL:H    | 4        | 0.2           |
| (1,1143) | 1:B:92:LYS:H    | 1:B:92:LYS:HA   | 5        | 0.2           |
| (1,1143) | 1:B:92:LYS:H    | 1:B:92:LYS:HA   | 6        | 0.2           |
| (1,1143) | 1:B:92:LYS:H    | 1:B:92:LYS:HA   | 7        | 0.2           |
| (1,1082) | 1:B:85:SER:HB3  | 1:B:89:LEU:H    | 2        | 0.2           |
| (1,1059) | 1:B:84:PHE:HD1  | 1:B:83:HIS:HB3  | 5        | 0.2           |
| (1,1059) | 1:B:84:PHE:HD2  | 1:B:83:HIS:HB3  | 5        | 0.2           |
| (1,1043) | 1:B:83:HIS:HB3  | 1:B:83:HIS:HD2  | 1        | 0.2           |
| (1,1033) | 1:B:81:VAL:HG11 | 1:B:118:PHE:HD1 | 9        | 0.2           |
| (1,1033) | 1:B:81:VAL:HG11 | 1:B:118:PHE:HD2 | 9        | 0.2           |
| (1,1033) | 1:B:81:VAL:HG12 | 1:B:118:PHE:HD1 | 9        | 0.2           |
| (1,1033) | 1:B:81:VAL:HG12 | 1:B:118:PHE:HD2 | 9        | 0.2           |
| (1,1033) | 1:B:81:VAL:HG13 | 1:B:118:PHE:HD1 | 9        | 0.2           |
| (1,1033) | 1:B:81:VAL:HG13 | 1:B:118:PHE:HD2 | 9        | 0.2           |
| (1,1031) | 1:B:81:VAL:HG21 | 1:B:84:PHE:H    | 4        | 0.2           |
| (1,1031) | 1:B:81:VAL:HG22 | 1:B:84:PHE:H    | 4        | 0.2           |
| (1,1031) | 1:B:81:VAL:HG23 | 1:B:84:PHE:H    | 4        | 0.2           |
| (1,1028) | 1:B:81:VAL:H    | 1:B:82:LYS:HA   | 4        | 0.2           |
| (1,995)  | 1:B:78:ASN:HA   | 1:B:79:LEU:H    | 4        | 0.19          |
| (1,988)  | 1:B:78:ASN:HA   | 1:B:78:ASN:HB2  | 3        | 0.19          |
| (1,988)  | 1:B:78:ASN:HA   | 1:B:78:ASN:HB2  | 4        | 0.19          |
| (1,975)  | 1:B:77:VAL:HG11 | 1:B:79:LEU:H    | 3        | 0.19          |
| (1,975)  | 1:B:77:VAL:HG12 | 1:B:79:LEU:H    | 3        | 0.19          |
| (1,975)  | 1:B:77:VAL:HG13 | 1:B:79:LEU:H    | 3        | 0.19          |
| (1,952)  | 1:B:77:VAL:HB   | 1:B:75:PHE:HD1  | 5        | 0.19          |
| (1,952)  | 1:B:77:VAL:HB   | 1:B:75:PHE:HD2  | 5        | 0.19          |
| (1,945)  | 1:B:76:SER:HA   | 1:B:146:ASP:HA  | 2        | 0.19          |
| (1,945)  | 1:B:76:SER:HA   | 1:B:146:ASP:HA  | 7        | 0.19          |
| (1,944)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB3 | 5        | 0.19          |
| (1,941)  | 1:B:76:SER:HA   | 1:B:146:ASP:HA  | 2        | 0.19          |
| (1,941)  | 1:B:76:SER:HA   | 1:B:146:ASP:HA  | 7        | 0.19          |
| (1,914)  | 1:B:75:PHE:HA   | 1:B:75:PHE:HD1  | 5        | 0.19          |
| (1,914)  | 1:B:75:PHE:HA   | 1:B:75:PHE:HD2  | 5        | 0.19          |
| (1,896)  | 1:B:72:LYS:HB2  | 1:B:72:LYS:H    | 6        | 0.19          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,896) | 1:B:72:LYS:HB3   | 1:B:72:LYS:H    | 6        | 0.19          |
| (1,892) | 1:B:71:GLU:H     | 1:B:71:GLU:HG2  | 7        | 0.19          |
| (1,892) | 1:B:71:GLU:H     | 1:B:71:GLU:HG3  | 7        | 0.19          |
| (1,891) | 1:B:71:GLU:H     | 1:B:69:ARG:HG2  | 7        | 0.19          |
| (1,891) | 1:B:71:GLU:H     | 1:B:69:ARG:HG3  | 7        | 0.19          |
| (1,876) | 1:B:68:MET:HE1   | 1:B:68:MET:H    | 9        | 0.19          |
| (1,876) | 1:B:68:MET:HE2   | 1:B:68:MET:H    | 9        | 0.19          |
| (1,876) | 1:B:68:MET:HE3   | 1:B:68:MET:H    | 9        | 0.19          |
| (1,85)  | 1:A:77:VAL:HB    | 1:A:75:PHE:HD1  | 5        | 0.19          |
| (1,85)  | 1:A:77:VAL:HB    | 1:A:75:PHE:HD2  | 5        | 0.19          |
| (1,847) | 1:A:147:GLY:HA2  | 1:A:147:GLY:H   | 3        | 0.19          |
| (1,835) | 1:A:146:ASP:HB2  | 1:A:146:ASP:HA  | 4        | 0.19          |
| (1,832) | 1:A:146:ASP:HB2  | 1:A:146:ASP:HA  | 4        | 0.19          |
| (1,827) | 1:A:146:ASP:HB3  | 1:A:76:SER:HA   | 6        | 0.19          |
| (1,825) | 1:A:146:ASP:HB2  | 1:A:76:SER:HA   | 8        | 0.19          |
| (1,824) | 1:A:146:ASP:HB2  | 1:A:76:SER:HA   | 8        | 0.19          |
| (1,816) | 1:A:145:VAL:HA   | 1:A:145:VAL:H   | 3        | 0.19          |
| (1,816) | 1:A:145:VAL:HA   | 1:A:145:VAL:H   | 8        | 0.19          |
| (1,809) | 1:A:144:THR:HG21 | 1:A:146:ASP:HB3 | 2        | 0.19          |
| (1,809) | 1:A:144:THR:HG22 | 1:A:146:ASP:HB3 | 2        | 0.19          |
| (1,809) | 1:A:144:THR:HG23 | 1:A:146:ASP:HB3 | 2        | 0.19          |
| (1,78)  | 1:A:76:SER:HA    | 1:A:146:ASP:HA  | 2        | 0.19          |
| (1,771) | 1:A:141:GLY:HA2  | 1:A:141:GLY:H   | 4        | 0.19          |
| (1,74)  | 1:A:76:SER:HA    | 1:A:146:ASP:HA  | 2        | 0.19          |
| (1,731) | 1:A:134:THR:HG21 | 1:A:135:SER:H   | 1        | 0.19          |
| (1,731) | 1:A:134:THR:HG22 | 1:A:135:SER:H   | 1        | 0.19          |
| (1,731) | 1:A:134:THR:HG23 | 1:A:135:SER:H   | 1        | 0.19          |
| (1,700) | 1:A:132:THR:HG21 | 1:A:132:THR:H   | 9        | 0.19          |
| (1,700) | 1:A:132:THR:HG22 | 1:A:132:THR:H   | 9        | 0.19          |
| (1,700) | 1:A:132:THR:HG23 | 1:A:132:THR:H   | 9        | 0.19          |
| (1,687) | 1:A:130:PRO:HG2  | 1:A:131:LEU:H   | 9        | 0.19          |
| (1,687) | 1:A:130:PRO:HG3  | 1:A:131:LEU:H   | 9        | 0.19          |
| (1,670) | 1:A:127:ASP:HB3  | 1:A:127:ASP:H   | 1        | 0.19          |
| (1,670) | 1:A:127:ASP:HB3  | 1:A:127:ASP:H   | 3        | 0.19          |
| (1,670) | 1:A:127:ASP:HB3  | 1:A:127:ASP:H   | 6        | 0.19          |
| (1,670) | 1:A:127:ASP:HB3  | 1:A:127:ASP:H   | 9        | 0.19          |
| (1,606) | 1:A:123:ARG:HB2  | 1:A:123:ARG:HD2 | 4        | 0.19          |
| (1,606) | 1:A:123:ARG:HB2  | 1:A:123:ARG:HD3 | 4        | 0.19          |
| (1,606) | 1:A:123:ARG:HB2  | 1:A:123:ARG:HD2 | 8        | 0.19          |
| (1,606) | 1:A:123:ARG:HB2  | 1:A:123:ARG:HD3 | 8        | 0.19          |
| (1,576) | 1:A:119:HIS:HB3  | 1:A:119:HIS:HA  | 3        | 0.19          |
| (1,576) | 1:A:119:HIS:HB3  | 1:A:119:HIS:HA  | 9        | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,575) | 1:A:119:HIS:HB3 | 1:A:119:HIS:HA  | 3        | 0.19          |
| (1,575) | 1:A:119:HIS:HB3 | 1:A:119:HIS:HA  | 9        | 0.19          |
| (1,506) | 1:A:114:ILE:HB  | 1:A:107:ARG:HD3 | 4        | 0.19          |
| (1,497) | 1:A:113:PHE:HD1 | 1:A:113:PHE:H   | 9        | 0.19          |
| (1,497) | 1:A:113:PHE:HD2 | 1:A:113:PHE:H   | 9        | 0.19          |
| (1,478) | 1:A:112:GLY:HA2 | 1:A:112:GLY:H   | 1        | 0.19          |
| (1,478) | 1:A:112:GLY:HA2 | 1:A:112:GLY:H   | 8        | 0.19          |
| (1,47)  | 1:A:75:PHE:HA   | 1:A:75:PHE:HD1  | 5        | 0.19          |
| (1,47)  | 1:A:75:PHE:HA   | 1:A:75:PHE:HD2  | 5        | 0.19          |
| (1,450) | 1:A:109:ASP:H   | 1:A:112:GLY:H   | 2        | 0.19          |
| (1,430) | 1:A:107:ARG:H   | 1:A:108:GLN:H   | 8        | 0.19          |
| (1,426) | 1:A:107:ARG:HD2 | 1:A:107:ARG:H   | 5        | 0.19          |
| (1,417) | 1:A:105:GLU:HG2 | 1:A:106:GLU:H   | 8        | 0.19          |
| (1,417) | 1:A:105:GLU:HG3 | 1:A:106:GLU:H   | 8        | 0.19          |
| (1,416) | 1:A:105:GLU:HG2 | 1:A:106:GLU:H   | 8        | 0.19          |
| (1,416) | 1:A:105:GLU:HG3 | 1:A:106:GLU:H   | 8        | 0.19          |
| (1,415) | 1:A:105:GLU:HA  | 1:A:106:GLU:H   | 7        | 0.19          |
| (1,383) | 1:A:101:HIS:HA  | 1:A:119:HIS:HD2 | 8        | 0.19          |
| (1,350) | 1:A:99:GLU:HA   | 1:A:98:ILE:HG21 | 9        | 0.19          |
| (1,350) | 1:A:99:GLU:HA   | 1:A:98:ILE:HG22 | 9        | 0.19          |
| (1,350) | 1:A:99:GLU:HA   | 1:A:98:ILE:HG23 | 9        | 0.19          |
| (1,339) | 1:A:98:ILE:HB   | 1:A:98:ILE:H    | 6        | 0.19          |
| (1,339) | 1:A:98:ILE:HB   | 1:A:98:ILE:H    | 8        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG11 | 3        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG12 | 3        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG13 | 3        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG21 | 3        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG22 | 3        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG23 | 3        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG11 | 9        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG12 | 9        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG13 | 9        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG21 | 9        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG22 | 9        | 0.19          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG23 | 9        | 0.19          |
| (1,297) | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD11 | 2        | 0.19          |
| (1,297) | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD12 | 2        | 0.19          |
| (1,297) | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD13 | 2        | 0.19          |
| (1,297) | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD21 | 2        | 0.19          |
| (1,297) | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD22 | 2        | 0.19          |
| (1,297) | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD23 | 2        | 0.19          |
| (1,29)  | 1:A:72:LYS:HB2  | 1:A:72:LYS:H    | 6        | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,29)   | 1:A:72:LYS:HB3   | 1:A:72:LYS:H    | 6        | 0.19          |
| (1,282)  | 1:A:93:VAL:H     | 1:A:92:LYS:HG2  | 2        | 0.19          |
| (1,282)  | 1:A:93:VAL:H     | 1:A:92:LYS:HG3  | 2        | 0.19          |
| (1,280)  | 1:A:92:LYS:H     | 1:A:100:VAL:HA  | 9        | 0.19          |
| (1,276)  | 1:A:92:LYS:H     | 1:A:92:LYS:HA   | 1        | 0.19          |
| (1,276)  | 1:A:92:LYS:H     | 1:A:92:LYS:HA   | 2        | 0.19          |
| (1,276)  | 1:A:92:LYS:H     | 1:A:92:LYS:HA   | 6        | 0.19          |
| (1,276)  | 1:A:92:LYS:H     | 1:A:92:LYS:HA   | 9        | 0.19          |
| (1,272)  | 1:A:92:LYS:H     | 1:A:91:VAL:HA   | 1        | 0.19          |
| (1,260)  | 1:A:89:LEU:HD21  | 1:A:103:LYS:H   | 2        | 0.19          |
| (1,260)  | 1:A:89:LEU:HD22  | 1:A:103:LYS:H   | 2        | 0.19          |
| (1,260)  | 1:A:89:LEU:HD23  | 1:A:103:LYS:H   | 2        | 0.19          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG2  | 7        | 0.19          |
| (1,25)   | 1:A:71:GLU:H     | 1:A:71:GLU:HG3  | 7        | 0.19          |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD21 | 1        | 0.19          |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD22 | 1        | 0.19          |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD23 | 1        | 0.19          |
| (1,228)  | 1:A:87:GLU:H     | 1:A:88:GLU:H    | 3        | 0.19          |
| (1,228)  | 1:A:87:GLU:H     | 1:A:88:GLU:H    | 8        | 0.19          |
| (1,225)  | 1:A:87:GLU:H     | 1:A:88:GLU:H    | 3        | 0.19          |
| (1,225)  | 1:A:87:GLU:H     | 1:A:88:GLU:H    | 8        | 0.19          |
| (1,175)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB3  | 3        | 0.19          |
| (1,174)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HB3  | 3        | 0.19          |
| (1,173)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HD2  | 7        | 0.19          |
| (1,1714) | 1:B:147:GLY:HA2  | 1:B:147:GLY:H   | 3        | 0.19          |
| (1,1702) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 4        | 0.19          |
| (1,170)  | 1:A:83:HIS:H     | 1:A:81:VAL:HB   | 3        | 0.19          |
| (1,1699) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 4        | 0.19          |
| (1,1694) | 1:B:146:ASP:HB3  | 1:B:76:SER:HA   | 6        | 0.19          |
| (1,1692) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA   | 8        | 0.19          |
| (1,1691) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA   | 8        | 0.19          |
| (1,1689) | 1:B:145:VAL:HA   | 1:B:146:ASP:H   | 2        | 0.19          |
| (1,1683) | 1:B:145:VAL:HA   | 1:B:145:VAL:H   | 3        | 0.19          |
| (1,1683) | 1:B:145:VAL:HA   | 1:B:145:VAL:H   | 7        | 0.19          |
| (1,1683) | 1:B:145:VAL:HA   | 1:B:145:VAL:H   | 8        | 0.19          |
| (1,1661) | 1:B:144:THR:HG21 | 1:B:78:ASN:HA   | 4        | 0.19          |
| (1,1661) | 1:B:144:THR:HG22 | 1:B:78:ASN:HA   | 4        | 0.19          |
| (1,1661) | 1:B:144:THR:HG23 | 1:B:78:ASN:HA   | 4        | 0.19          |
| (1,1638) | 1:B:141:GLY:HA2  | 1:B:141:GLY:H   | 4        | 0.19          |
| (1,1598) | 1:B:134:THR:HG21 | 1:B:135:SER:H   | 1        | 0.19          |
| (1,1598) | 1:B:134:THR:HG22 | 1:B:135:SER:H   | 1        | 0.19          |
| (1,1598) | 1:B:134:THR:HG23 | 1:B:135:SER:H   | 1        | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1567) | 1:B:132:THR:HG21 | 1:B:132:THR:H   | 9        | 0.19          |
| (1,1567) | 1:B:132:THR:HG22 | 1:B:132:THR:H   | 9        | 0.19          |
| (1,1567) | 1:B:132:THR:HG23 | 1:B:132:THR:H   | 9        | 0.19          |
| (1,1537) | 1:B:127:ASP:HB3  | 1:B:127:ASP:H   | 1        | 0.19          |
| (1,1537) | 1:B:127:ASP:HB3  | 1:B:127:ASP:H   | 3        | 0.19          |
| (1,1473) | 1:B:123:ARG:HB2  | 1:B:123:ARG:HD2 | 4        | 0.19          |
| (1,1473) | 1:B:123:ARG:HB2  | 1:B:123:ARG:HD3 | 4        | 0.19          |
| (1,1473) | 1:B:123:ARG:HB2  | 1:B:123:ARG:HD2 | 8        | 0.19          |
| (1,1473) | 1:B:123:ARG:HB2  | 1:B:123:ARG:HD3 | 8        | 0.19          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG21 | 2        | 0.19          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG22 | 2        | 0.19          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG23 | 2        | 0.19          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG21 | 2        | 0.19          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG22 | 2        | 0.19          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG23 | 2        | 0.19          |
| (1,1443) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA  | 3        | 0.19          |
| (1,1443) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA  | 9        | 0.19          |
| (1,1442) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA  | 3        | 0.19          |
| (1,1442) | 1:B:119:HIS:HB3  | 1:B:119:HIS:HA  | 9        | 0.19          |
| (1,138)  | 1:A:79:LEU:HD11  | 1:A:79:LEU:HA   | 1        | 0.19          |
| (1,138)  | 1:A:79:LEU:HD12  | 1:A:79:LEU:HA   | 1        | 0.19          |
| (1,138)  | 1:A:79:LEU:HD13  | 1:A:79:LEU:HA   | 1        | 0.19          |
| (1,138)  | 1:A:79:LEU:HD21  | 1:A:79:LEU:HA   | 1        | 0.19          |
| (1,138)  | 1:A:79:LEU:HD22  | 1:A:79:LEU:HA   | 1        | 0.19          |
| (1,138)  | 1:A:79:LEU:HD23  | 1:A:79:LEU:HA   | 1        | 0.19          |
| (1,1373) | 1:B:114:ILE:HB   | 1:B:107:ARG:HD3 | 4        | 0.19          |
| (1,1364) | 1:B:113:PHE:HD1  | 1:B:113:PHE:H   | 9        | 0.19          |
| (1,1364) | 1:B:113:PHE:HD2  | 1:B:113:PHE:H   | 9        | 0.19          |
| (1,1345) | 1:B:112:GLY:HA2  | 1:B:112:GLY:H   | 1        | 0.19          |
| (1,1345) | 1:B:112:GLY:HA2  | 1:B:112:GLY:H   | 8        | 0.19          |
| (1,1331) | 1:B:111:HIS:H    | 1:B:111:HIS:HD2 | 8        | 0.19          |
| (1,1317) | 1:B:109:ASP:H    | 1:B:112:GLY:H   | 2        | 0.19          |
| (1,1297) | 1:B:107:ARG:H    | 1:B:108:GLN:H   | 8        | 0.19          |
| (1,1293) | 1:B:107:ARG:HD2  | 1:B:107:ARG:H   | 5        | 0.19          |
| (1,1284) | 1:B:105:GLU:HG2  | 1:B:106:GLU:H   | 8        | 0.19          |
| (1,1284) | 1:B:105:GLU:HG3  | 1:B:106:GLU:H   | 8        | 0.19          |
| (1,1283) | 1:B:105:GLU:HG2  | 1:B:106:GLU:H   | 8        | 0.19          |
| (1,1283) | 1:B:105:GLU:HG3  | 1:B:106:GLU:H   | 8        | 0.19          |
| (1,128)  | 1:A:78:ASN:HA    | 1:A:79:LEU:H    | 4        | 0.19          |
| (1,127)  | 1:A:78:ASN:HA    | 1:A:79:LEU:HD11 | 5        | 0.19          |
| (1,127)  | 1:A:78:ASN:HA    | 1:A:79:LEU:HD12 | 5        | 0.19          |
| (1,127)  | 1:A:78:ASN:HA    | 1:A:79:LEU:HD13 | 5        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD21 | 5        | 0.19          |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD22 | 5        | 0.19          |
| (1,127)  | 1:A:78:ASN:HA   | 1:A:79:LEU:HD23 | 5        | 0.19          |
| (1,1250) | 1:B:101:HIS:HA  | 1:B:119:HIS:HD2 | 8        | 0.19          |
| (1,1245) | 1:B:101:HIS:HB3 | 1:B:101:HIS:H   | 9        | 0.19          |
| (1,1217) | 1:B:99:GLU:HA   | 1:B:98:ILE:HG21 | 9        | 0.19          |
| (1,1217) | 1:B:99:GLU:HA   | 1:B:98:ILE:HG22 | 9        | 0.19          |
| (1,1217) | 1:B:99:GLU:HA   | 1:B:98:ILE:HG23 | 9        | 0.19          |
| (1,121)  | 1:A:78:ASN:HA   | 1:A:78:ASN:HB2  | 3        | 0.19          |
| (1,121)  | 1:A:78:ASN:HA   | 1:A:78:ASN:HB2  | 4        | 0.19          |
| (1,121)  | 1:A:78:ASN:HA   | 1:A:78:ASN:HB2  | 5        | 0.19          |
| (1,1206) | 1:B:98:ILE:HB   | 1:B:98:ILE:H    | 6        | 0.19          |
| (1,1206) | 1:B:98:ILE:HB   | 1:B:98:ILE:H    | 8        | 0.19          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG11 | 9        | 0.19          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG12 | 9        | 0.19          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG13 | 9        | 0.19          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG21 | 9        | 0.19          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG22 | 9        | 0.19          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG23 | 9        | 0.19          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD11 | 2        | 0.19          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD12 | 2        | 0.19          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD13 | 2        | 0.19          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD21 | 2        | 0.19          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD22 | 2        | 0.19          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD23 | 2        | 0.19          |
| (1,1149) | 1:B:93:VAL:H    | 1:B:92:LYS:HG2  | 2        | 0.19          |
| (1,1149) | 1:B:93:VAL:H    | 1:B:92:LYS:HG3  | 2        | 0.19          |
| (1,1147) | 1:B:92:LYS:H    | 1:B:100:VAL:HA  | 9        | 0.19          |
| (1,1143) | 1:B:92:LYS:H    | 1:B:92:LYS:HA   | 1        | 0.19          |
| (1,1143) | 1:B:92:LYS:H    | 1:B:92:LYS:HA   | 2        | 0.19          |
| (1,1143) | 1:B:92:LYS:H    | 1:B:92:LYS:HA   | 3        | 0.19          |
| (1,1143) | 1:B:92:LYS:H    | 1:B:92:LYS:HA   | 9        | 0.19          |
| (1,1139) | 1:B:92:LYS:H    | 1:B:91:VAL:HA   | 1        | 0.19          |
| (1,1127) | 1:B:89:LEU:HD21 | 1:B:103:LYS:H   | 2        | 0.19          |
| (1,1127) | 1:B:89:LEU:HD22 | 1:B:103:LYS:H   | 2        | 0.19          |
| (1,1127) | 1:B:89:LEU:HD23 | 1:B:103:LYS:H   | 2        | 0.19          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD21 | 1        | 0.19          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD22 | 1        | 0.19          |
| (1,1112) | 1:B:89:LEU:HA   | 1:B:89:LEU:HD23 | 1        | 0.19          |
| (1,1095) | 1:B:87:GLU:H    | 1:B:88:GLU:H    | 3        | 0.19          |
| (1,1095) | 1:B:87:GLU:H    | 1:B:88:GLU:H    | 8        | 0.19          |
| (1,1092) | 1:B:87:GLU:H    | 1:B:88:GLU:H    | 3        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1092) | 1:B:87:GLU:H    | 1:B:88:GLU:H    | 8        | 0.19          |
| (1,108)  | 1:A:77:VAL:HG11 | 1:A:79:LEU:H    | 3        | 0.19          |
| (1,108)  | 1:A:77:VAL:HG12 | 1:A:79:LEU:H    | 3        | 0.19          |
| (1,108)  | 1:A:77:VAL:HG13 | 1:A:79:LEU:H    | 3        | 0.19          |
| (1,1042) | 1:B:83:HIS:HA   | 1:B:83:HIS:HB3  | 3        | 0.19          |
| (1,1041) | 1:B:83:HIS:HA   | 1:B:83:HIS:HB3  | 3        | 0.19          |
| (1,1037) | 1:B:83:HIS:H    | 1:B:81:VAL:HB   | 3        | 0.19          |
| (1,1005) | 1:B:79:LEU:HD11 | 1:B:79:LEU:HA   | 1        | 0.19          |
| (1,1005) | 1:B:79:LEU:HD12 | 1:B:79:LEU:HA   | 1        | 0.19          |
| (1,1005) | 1:B:79:LEU:HD13 | 1:B:79:LEU:HA   | 1        | 0.19          |
| (1,1005) | 1:B:79:LEU:HD21 | 1:B:79:LEU:HA   | 1        | 0.19          |
| (1,1005) | 1:B:79:LEU:HD22 | 1:B:79:LEU:HA   | 1        | 0.19          |
| (1,1005) | 1:B:79:LEU:HD23 | 1:B:79:LEU:HA   | 1        | 0.19          |
| (1,996)  | 1:B:78:ASN:HB3  | 1:B:79:LEU:H    | 2        | 0.18          |
| (1,996)  | 1:B:78:ASN:HB3  | 1:B:79:LEU:H    | 9        | 0.18          |
| (1,994)  | 1:B:78:ASN:HA   | 1:B:79:LEU:HD11 | 5        | 0.18          |
| (1,994)  | 1:B:78:ASN:HA   | 1:B:79:LEU:HD12 | 5        | 0.18          |
| (1,994)  | 1:B:78:ASN:HA   | 1:B:79:LEU:HD13 | 5        | 0.18          |
| (1,994)  | 1:B:78:ASN:HA   | 1:B:79:LEU:HD21 | 5        | 0.18          |
| (1,994)  | 1:B:78:ASN:HA   | 1:B:79:LEU:HD22 | 5        | 0.18          |
| (1,994)  | 1:B:78:ASN:HA   | 1:B:79:LEU:HD23 | 5        | 0.18          |
| (1,988)  | 1:B:78:ASN:HA   | 1:B:78:ASN:HB2  | 2        | 0.18          |
| (1,970)  | 1:B:77:VAL:H    | 1:B:78:ASN:H    | 8        | 0.18          |
| (1,952)  | 1:B:77:VAL:HB   | 1:B:75:PHE:HD1  | 3        | 0.18          |
| (1,952)  | 1:B:77:VAL:HB   | 1:B:75:PHE:HD2  | 3        | 0.18          |
| (1,923)  | 1:B:75:PHE:HD1  | 1:B:148:PRO:HA  | 7        | 0.18          |
| (1,923)  | 1:B:75:PHE:HD2  | 1:B:148:PRO:HA  | 7        | 0.18          |
| (1,921)  | 1:B:75:PHE:HD1  | 1:B:146:ASP:HB3 | 1        | 0.18          |
| (1,921)  | 1:B:75:PHE:HD2  | 1:B:146:ASP:HB3 | 1        | 0.18          |
| (1,895)  | 1:B:72:LYS:H    | 1:B:72:LYS:HA   | 7        | 0.18          |
| (1,863)  | 1:A:150:LYS:H   | 1:A:151:GLN:H   | 3        | 0.18          |
| (1,860)  | 1:A:150:LYS:H   | 1:A:151:GLN:H   | 3        | 0.18          |
| (1,856)  | 1:A:150:LYS:H   | 1:A:149:ARG:H   | 5        | 0.18          |
| (1,854)  | 1:A:148:PRO:HB2 | 1:A:149:ARG:H   | 4        | 0.18          |
| (1,854)  | 1:A:148:PRO:HB3 | 1:A:149:ARG:H   | 4        | 0.18          |
| (1,85)   | 1:A:77:VAL:HB   | 1:A:75:PHE:HD1  | 3        | 0.18          |
| (1,85)   | 1:A:77:VAL:HB   | 1:A:75:PHE:HD2  | 3        | 0.18          |
| (1,835)  | 1:A:146:ASP:HB2 | 1:A:146:ASP:HA  | 2        | 0.18          |
| (1,835)  | 1:A:146:ASP:HB2 | 1:A:146:ASP:HA  | 7        | 0.18          |
| (1,835)  | 1:A:146:ASP:HB2 | 1:A:146:ASP:HA  | 8        | 0.18          |
| (1,832)  | 1:A:146:ASP:HB2 | 1:A:146:ASP:HA  | 2        | 0.18          |
| (1,832)  | 1:A:146:ASP:HB2 | 1:A:146:ASP:HA  | 7        | 0.18          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,832) | 1:A:146:ASP:HB2  | 1:A:146:ASP:HA  | 8        | 0.18          |
| (1,822) | 1:A:145:VAL:HA   | 1:A:146:ASP:H   | 5        | 0.18          |
| (1,820) | 1:A:145:VAL:HG11 | 1:A:146:ASP:HB2 | 5        | 0.18          |
| (1,820) | 1:A:145:VAL:HG12 | 1:A:146:ASP:HB2 | 5        | 0.18          |
| (1,820) | 1:A:145:VAL:HG13 | 1:A:146:ASP:HB2 | 5        | 0.18          |
| (1,817) | 1:A:145:VAL:HB   | 1:A:145:VAL:H   | 4        | 0.18          |
| (1,817) | 1:A:145:VAL:HB   | 1:A:145:VAL:H   | 7        | 0.18          |
| (1,802) | 1:A:144:THR:HB   | 1:A:144:THR:H   | 8        | 0.18          |
| (1,794) | 1:A:144:THR:HG21 | 1:A:78:ASN:HA   | 5        | 0.18          |
| (1,794) | 1:A:144:THR:HG22 | 1:A:78:ASN:HA   | 5        | 0.18          |
| (1,794) | 1:A:144:THR:HG23 | 1:A:78:ASN:HA   | 5        | 0.18          |
| (1,746) | 1:A:136:SER:H    | 1:A:135:SER:H   | 1        | 0.18          |
| (1,705) | 1:A:132:THR:HG1  | 1:A:133:ILE:H   | 7        | 0.18          |
| (1,681) | 1:A:128:VAL:H    | 1:A:150:LYS:HD2 | 2        | 0.18          |
| (1,681) | 1:A:128:VAL:H    | 1:A:150:LYS:HD3 | 2        | 0.18          |
| (1,680) | 1:A:128:VAL:H    | 1:A:129:ASP:H   | 5        | 0.18          |
| (1,670) | 1:A:127:ASP:HB3  | 1:A:127:ASP:H   | 8        | 0.18          |
| (1,643) | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD1 | 4        | 0.18          |
| (1,643) | 1:A:125:PRO:HD2  | 1:A:122:TYR:HD2 | 4        | 0.18          |
| (1,616) | 1:A:124:ILE:HD11 | 1:A:97:VAL:H    | 6        | 0.18          |
| (1,616) | 1:A:124:ILE:HD12 | 1:A:97:VAL:H    | 6        | 0.18          |
| (1,616) | 1:A:124:ILE:HD13 | 1:A:97:VAL:H    | 6        | 0.18          |
| (1,590) | 1:A:122:TYR:HA   | 1:A:98:ILE:H    | 2        | 0.18          |
| (1,572) | 1:A:119:HIS:HB2  | 1:A:119:HIS:HA  | 8        | 0.18          |
| (1,56)  | 1:A:75:PHE:HD1   | 1:A:148:PRO:HA  | 7        | 0.18          |
| (1,56)  | 1:A:75:PHE:HD2   | 1:A:148:PRO:HA  | 7        | 0.18          |
| (1,54)  | 1:A:75:PHE:HD1   | 1:A:146:ASP:HB3 | 1        | 0.18          |
| (1,54)  | 1:A:75:PHE:HD2   | 1:A:146:ASP:HB3 | 1        | 0.18          |
| (1,535) | 1:A:116:ARG:H    | 1:A:104:HIS:H   | 4        | 0.18          |
| (1,534) | 1:A:116:ARG:H    | 1:A:104:HIS:H   | 4        | 0.18          |
| (1,533) | 1:A:115:SER:HB2  | 1:A:116:ARG:H   | 9        | 0.18          |
| (1,482) | 1:A:113:PHE:HD1  | 1:A:107:ARG:HA  | 2        | 0.18          |
| (1,482) | 1:A:113:PHE:HD2  | 1:A:107:ARG:HA  | 2        | 0.18          |
| (1,478) | 1:A:112:GLY:HA2  | 1:A:112:GLY:H   | 2        | 0.18          |
| (1,454) | 1:A:110:GLU:H    | 1:A:110:GLU:HA  | 1        | 0.18          |
| (1,445) | 1:A:108:GLN:HA   | 1:A:113:PHE:H   | 5        | 0.18          |
| (1,427) | 1:A:107:ARG:HB3  | 1:A:107:ARG:H   | 1        | 0.18          |
| (1,425) | 1:A:107:ARG:HA   | 1:A:107:ARG:H   | 5        | 0.18          |
| (1,390) | 1:A:102:GLY:HA2  | 1:A:103:LYS:H   | 4        | 0.18          |
| (1,379) | 1:A:101:HIS:HB2  | 1:A:101:HIS:H   | 4        | 0.18          |
| (1,378) | 1:A:101:HIS:HB3  | 1:A:101:HIS:H   | 9        | 0.18          |
| (1,369) | 1:A:101:HIS:H    | 1:A:100:VAL:HA  | 5        | 0.18          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,368)  | 1:A:101:HIS:HB2  | 1:A:92:LYS:HB2  | 4        | 0.18          |
| (1,368)  | 1:A:101:HIS:HB2  | 1:A:92:LYS:HB3  | 4        | 0.18          |
| (1,330)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA  | 7        | 0.18          |
| (1,329)  | 1:A:97:VAL:HA    | 1:A:123:ARG:HA  | 7        | 0.18          |
| (1,28)   | 1:A:72:LYS:H     | 1:A:72:LYS:HA   | 7        | 0.18          |
| (1,254)  | 1:A:89:LEU:HD11  | 1:A:91:VAL:HB   | 5        | 0.18          |
| (1,254)  | 1:A:89:LEU:HD12  | 1:A:91:VAL:HB   | 5        | 0.18          |
| (1,254)  | 1:A:89:LEU:HD13  | 1:A:91:VAL:HB   | 5        | 0.18          |
| (1,248)  | 1:A:89:LEU:HD11  | 1:A:89:LEU:H    | 3        | 0.18          |
| (1,248)  | 1:A:89:LEU:HD12  | 1:A:89:LEU:H    | 3        | 0.18          |
| (1,248)  | 1:A:89:LEU:HD13  | 1:A:89:LEU:H    | 3        | 0.18          |
| (1,228)  | 1:A:87:GLU:H     | 1:A:88:GLU:H    | 7        | 0.18          |
| (1,225)  | 1:A:87:GLU:H     | 1:A:88:GLU:H    | 7        | 0.18          |
| (1,191)  | 1:A:84:PHE:HD1   | 1:A:82:LYS:H    | 2        | 0.18          |
| (1,191)  | 1:A:84:PHE:HD2   | 1:A:82:LYS:H    | 2        | 0.18          |
| (1,1730) | 1:B:150:LYS:H    | 1:B:151:GLN:H   | 3        | 0.18          |
| (1,1727) | 1:B:150:LYS:H    | 1:B:151:GLN:H   | 3        | 0.18          |
| (1,1721) | 1:B:148:PRO:HB2  | 1:B:149:ARG:H   | 4        | 0.18          |
| (1,1721) | 1:B:148:PRO:HB3  | 1:B:149:ARG:H   | 4        | 0.18          |
| (1,1702) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 2        | 0.18          |
| (1,1702) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 7        | 0.18          |
| (1,1702) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 8        | 0.18          |
| (1,1699) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 2        | 0.18          |
| (1,1699) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 7        | 0.18          |
| (1,1699) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 8        | 0.18          |
| (1,1692) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA   | 4        | 0.18          |
| (1,1691) | 1:B:146:ASP:HB2  | 1:B:76:SER:HA   | 4        | 0.18          |
| (1,1689) | 1:B:145:VAL:HA   | 1:B:146:ASP:H   | 5        | 0.18          |
| (1,1687) | 1:B:145:VAL:HG11 | 1:B:146:ASP:HB2 | 5        | 0.18          |
| (1,1687) | 1:B:145:VAL:HG12 | 1:B:146:ASP:HB2 | 5        | 0.18          |
| (1,1687) | 1:B:145:VAL:HG13 | 1:B:146:ASP:HB2 | 5        | 0.18          |
| (1,1684) | 1:B:145:VAL:HB   | 1:B:145:VAL:H   | 7        | 0.18          |
| (1,1676) | 1:B:144:THR:HG21 | 1:B:146:ASP:HB3 | 2        | 0.18          |
| (1,1676) | 1:B:144:THR:HG22 | 1:B:146:ASP:HB3 | 2        | 0.18          |
| (1,1676) | 1:B:144:THR:HG23 | 1:B:146:ASP:HB3 | 2        | 0.18          |
| (1,1669) | 1:B:144:THR:HB   | 1:B:144:THR:H   | 8        | 0.18          |
| (1,1661) | 1:B:144:THR:HG21 | 1:B:78:ASN:HA   | 5        | 0.18          |
| (1,1661) | 1:B:144:THR:HG22 | 1:B:78:ASN:HA   | 5        | 0.18          |
| (1,1661) | 1:B:144:THR:HG23 | 1:B:78:ASN:HA   | 5        | 0.18          |
| (1,1613) | 1:B:136:SER:H    | 1:B:135:SER:H   | 1        | 0.18          |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD2 | 2        | 0.18          |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD3 | 2        | 0.18          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1547) | 1:B:128:VAL:H    | 1:B:129:ASP:H   | 5        | 0.18          |
| (1,1537) | 1:B:127:ASP:HB3  | 1:B:127:ASP:H   | 6        | 0.18          |
| (1,1537) | 1:B:127:ASP:HB3  | 1:B:127:ASP:H   | 8        | 0.18          |
| (1,1537) | 1:B:127:ASP:HB3  | 1:B:127:ASP:H   | 9        | 0.18          |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD1 | 4        | 0.18          |
| (1,1510) | 1:B:125:PRO:HD2  | 1:B:122:TYR:HD2 | 4        | 0.18          |
| (1,1483) | 1:B:124:ILE:HD11 | 1:B:97:VAL:H    | 6        | 0.18          |
| (1,1483) | 1:B:124:ILE:HD12 | 1:B:97:VAL:H    | 6        | 0.18          |
| (1,1483) | 1:B:124:ILE:HD13 | 1:B:97:VAL:H    | 6        | 0.18          |
| (1,148)  | 1:A:80:ASP:H     | 1:A:80:ASP:HB3  | 6        | 0.18          |
| (1,148)  | 1:A:80:ASP:H     | 1:A:80:ASP:HB3  | 7        | 0.18          |
| (1,1457) | 1:B:122:TYR:HA   | 1:B:98:ILE:H    | 2        | 0.18          |
| (1,1439) | 1:B:119:HIS:HB2  | 1:B:119:HIS:HA  | 8        | 0.18          |
| (1,1402) | 1:B:116:ARG:H    | 1:B:104:HIS:H   | 4        | 0.18          |
| (1,1401) | 1:B:116:ARG:H    | 1:B:104:HIS:H   | 4        | 0.18          |
| (1,1400) | 1:B:115:SER:HB2  | 1:B:116:ARG:H   | 9        | 0.18          |
| (1,1349) | 1:B:113:PHE:HD1  | 1:B:107:ARG:HA  | 2        | 0.18          |
| (1,1349) | 1:B:113:PHE:HD2  | 1:B:107:ARG:HA  | 2        | 0.18          |
| (1,1345) | 1:B:112:GLY:HA2  | 1:B:112:GLY:H   | 2        | 0.18          |
| (1,1321) | 1:B:110:GLU:H    | 1:B:110:GLU:HA  | 1        | 0.18          |
| (1,1312) | 1:B:108:GLN:HA   | 1:B:113:PHE:H   | 5        | 0.18          |
| (1,1294) | 1:B:107:ARG:HB3  | 1:B:107:ARG:H   | 1        | 0.18          |
| (1,1292) | 1:B:107:ARG:HA   | 1:B:107:ARG:H   | 5        | 0.18          |
| (1,129)  | 1:A:78:ASN:HB3   | 1:A:79:LEU:H    | 2        | 0.18          |
| (1,129)  | 1:A:78:ASN:HB3   | 1:A:79:LEU:H    | 9        | 0.18          |
| (1,1257) | 1:B:102:GLY:HA2  | 1:B:103:LYS:H   | 4        | 0.18          |
| (1,1246) | 1:B:101:HIS:HB2  | 1:B:101:HIS:H   | 4        | 0.18          |
| (1,1236) | 1:B:101:HIS:H    | 1:B:100:VAL:HA  | 5        | 0.18          |
| (1,1235) | 1:B:101:HIS:HB2  | 1:B:92:LYS:HB2  | 4        | 0.18          |
| (1,1235) | 1:B:101:HIS:HB2  | 1:B:92:LYS:HB3  | 4        | 0.18          |
| (1,121)  | 1:A:78:ASN:HA    | 1:A:78:ASN:HB2  | 2        | 0.18          |
| (1,1197) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 7        | 0.18          |
| (1,1196) | 1:B:97:VAL:HA    | 1:B:123:ARG:HA  | 7        | 0.18          |
| (1,1121) | 1:B:89:LEU:HD11  | 1:B:91:VAL:HB   | 5        | 0.18          |
| (1,1121) | 1:B:89:LEU:HD12  | 1:B:91:VAL:HB   | 5        | 0.18          |
| (1,1121) | 1:B:89:LEU:HD13  | 1:B:91:VAL:HB   | 5        | 0.18          |
| (1,1115) | 1:B:89:LEU:HD11  | 1:B:89:LEU:H    | 3        | 0.18          |
| (1,1115) | 1:B:89:LEU:HD12  | 1:B:89:LEU:H    | 3        | 0.18          |
| (1,1115) | 1:B:89:LEU:HD13  | 1:B:89:LEU:H    | 3        | 0.18          |
| (1,1095) | 1:B:87:GLU:H     | 1:B:88:GLU:H    | 7        | 0.18          |
| (1,1092) | 1:B:87:GLU:H     | 1:B:88:GLU:H    | 7        | 0.18          |
| (1,1058) | 1:B:84:PHE:HD1   | 1:B:82:LYS:H    | 2        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1058) | 1:B:84:PHE:HD2  | 1:B:82:LYS:H    | 2        | 0.18          |
| (1,1040) | 1:B:83:HIS:HA   | 1:B:83:HIS:HD2  | 5        | 0.18          |
| (1,1040) | 1:B:83:HIS:HA   | 1:B:83:HIS:HD2  | 7        | 0.18          |
| (1,103)  | 1:A:77:VAL:H    | 1:A:78:ASN:H    | 8        | 0.18          |
| (1,1024) | 1:B:81:VAL:HG21 | 1:B:81:VAL:H    | 4        | 0.18          |
| (1,1024) | 1:B:81:VAL:HG22 | 1:B:81:VAL:H    | 4        | 0.18          |
| (1,1024) | 1:B:81:VAL:HG23 | 1:B:81:VAL:H    | 4        | 0.18          |
| (1,1015) | 1:B:80:ASP:H    | 1:B:80:ASP:HB3  | 6        | 0.18          |
| (1,1015) | 1:B:80:ASP:H    | 1:B:80:ASP:HB3  | 7        | 0.18          |
| (1,997)  | 1:B:78:ASN:HB2  | 1:B:79:LEU:H    | 8        | 0.17          |
| (1,982)  | 1:B:77:VAL:HG11 | 1:B:145:VAL:H   | 8        | 0.17          |
| (1,982)  | 1:B:77:VAL:HG12 | 1:B:145:VAL:H   | 8        | 0.17          |
| (1,982)  | 1:B:77:VAL:HG13 | 1:B:145:VAL:H   | 8        | 0.17          |
| (1,979)  | 1:B:77:VAL:HG11 | 1:B:122:TYR:HD1 | 7        | 0.17          |
| (1,979)  | 1:B:77:VAL:HG11 | 1:B:122:TYR:HD2 | 7        | 0.17          |
| (1,979)  | 1:B:77:VAL:HG12 | 1:B:122:TYR:HD1 | 7        | 0.17          |
| (1,979)  | 1:B:77:VAL:HG12 | 1:B:122:TYR:HD2 | 7        | 0.17          |
| (1,979)  | 1:B:77:VAL:HG13 | 1:B:122:TYR:HD1 | 7        | 0.17          |
| (1,979)  | 1:B:77:VAL:HG13 | 1:B:122:TYR:HD2 | 7        | 0.17          |
| (1,970)  | 1:B:77:VAL:H    | 1:B:78:ASN:H    | 4        | 0.17          |
| (1,896)  | 1:B:72:LYS:HB2  | 1:B:72:LYS:H    | 1        | 0.17          |
| (1,896)  | 1:B:72:LYS:HB3  | 1:B:72:LYS:H    | 1        | 0.17          |
| (1,896)  | 1:B:72:LYS:HB2  | 1:B:72:LYS:H    | 5        | 0.17          |
| (1,896)  | 1:B:72:LYS:HB3  | 1:B:72:LYS:H    | 5        | 0.17          |
| (1,895)  | 1:B:72:LYS:H    | 1:B:72:LYS:HA   | 9        | 0.17          |
| (1,872)  | 1:B:67:GLU:H    | 1:B:67:GLU:HA   | 2        | 0.17          |
| (1,872)  | 1:B:67:GLU:H    | 1:B:67:GLU:HA   | 3        | 0.17          |
| (1,872)  | 1:B:67:GLU:H    | 1:B:67:GLU:HA   | 8        | 0.17          |
| (1,856)  | 1:A:150:LYS:H   | 1:A:149:ARG:H   | 9        | 0.17          |
| (1,854)  | 1:A:148:PRO:HB2 | 1:A:149:ARG:H   | 3        | 0.17          |
| (1,854)  | 1:A:148:PRO:HB3 | 1:A:149:ARG:H   | 3        | 0.17          |
| (1,835)  | 1:A:146:ASP:HB2 | 1:A:146:ASP:HA  | 1        | 0.17          |
| (1,835)  | 1:A:146:ASP:HB2 | 1:A:146:ASP:HA  | 5        | 0.17          |
| (1,832)  | 1:A:146:ASP:HB2 | 1:A:146:ASP:HA  | 1        | 0.17          |
| (1,832)  | 1:A:146:ASP:HB2 | 1:A:146:ASP:HA  | 5        | 0.17          |
| (1,825)  | 1:A:146:ASP:HB2 | 1:A:76:SER:HA   | 4        | 0.17          |
| (1,824)  | 1:A:146:ASP:HB2 | 1:A:76:SER:HA   | 4        | 0.17          |
| (1,822)  | 1:A:145:VAL:HA  | 1:A:146:ASP:H   | 6        | 0.17          |
| (1,708)  | 1:A:132:THR:H   | 1:A:133:ILE:H   | 4        | 0.17          |
| (1,706)  | 1:A:132:THR:H   | 1:A:133:ILE:H   | 4        | 0.17          |
| (1,680)  | 1:A:128:VAL:H   | 1:A:129:ASP:H   | 3        | 0.17          |
| (1,680)  | 1:A:128:VAL:H   | 1:A:129:ASP:H   | 9        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,670) | 1:A:127:ASP:HB3 | 1:A:127:ASP:H   | 5        | 0.17          |
| (1,670) | 1:A:127:ASP:HB3 | 1:A:127:ASP:H   | 7        | 0.17          |
| (1,660) | 1:A:126:ALA:HA  | 1:A:128:VAL:H   | 7        | 0.17          |
| (1,656) | 1:A:125:PRO:HA  | 1:A:127:ASP:H   | 6        | 0.17          |
| (1,650) | 1:A:125:PRO:HD3 | 1:A:124:ILE:HB  | 4        | 0.17          |
| (1,606) | 1:A:123:ARG:HB2 | 1:A:123:ARG:HD2 | 5        | 0.17          |
| (1,606) | 1:A:123:ARG:HB2 | 1:A:123:ARG:HD3 | 5        | 0.17          |
| (1,606) | 1:A:123:ARG:HB2 | 1:A:123:ARG:HD2 | 9        | 0.17          |
| (1,606) | 1:A:123:ARG:HB2 | 1:A:123:ARG:HD3 | 9        | 0.17          |
| (1,593) | 1:A:122:TYR:HB2 | 1:A:122:TYR:HA  | 5        | 0.17          |
| (1,593) | 1:A:122:TYR:HB3 | 1:A:122:TYR:HA  | 5        | 0.17          |
| (1,591) | 1:A:122:TYR:HB2 | 1:A:122:TYR:HA  | 5        | 0.17          |
| (1,591) | 1:A:122:TYR:HB3 | 1:A:122:TYR:HA  | 5        | 0.17          |
| (1,588) | 1:A:122:TYR:HB2 | 1:A:98:ILE:HD11 | 1        | 0.17          |
| (1,588) | 1:A:122:TYR:HB2 | 1:A:98:ILE:HD12 | 1        | 0.17          |
| (1,588) | 1:A:122:TYR:HB2 | 1:A:98:ILE:HD13 | 1        | 0.17          |
| (1,588) | 1:A:122:TYR:HB3 | 1:A:98:ILE:HD11 | 1        | 0.17          |
| (1,588) | 1:A:122:TYR:HB3 | 1:A:98:ILE:HD12 | 1        | 0.17          |
| (1,588) | 1:A:122:TYR:HB3 | 1:A:98:ILE:HD13 | 1        | 0.17          |
| (1,5)   | 1:A:67:GLU:H    | 1:A:67:GLU:HA   | 2        | 0.17          |
| (1,5)   | 1:A:67:GLU:H    | 1:A:67:GLU:HA   | 3        | 0.17          |
| (1,5)   | 1:A:67:GLU:H    | 1:A:67:GLU:HA   | 8        | 0.17          |
| (1,471) | 1:A:111:HIS:H   | 1:A:112:GLY:H   | 3        | 0.17          |
| (1,468) | 1:A:111:HIS:H   | 1:A:112:GLY:H   | 3        | 0.17          |
| (1,454) | 1:A:110:GLU:H   | 1:A:110:GLU:HA  | 3        | 0.17          |
| (1,454) | 1:A:110:GLU:H   | 1:A:110:GLU:HA  | 7        | 0.17          |
| (1,454) | 1:A:110:GLU:H   | 1:A:110:GLU:HA  | 9        | 0.17          |
| (1,430) | 1:A:107:ARG:H   | 1:A:108:GLN:H   | 1        | 0.17          |
| (1,430) | 1:A:107:ARG:H   | 1:A:108:GLN:H   | 5        | 0.17          |
| (1,418) | 1:A:105:GLU:HG2 | 1:A:115:SER:HB3 | 7        | 0.17          |
| (1,418) | 1:A:105:GLU:HG3 | 1:A:115:SER:HB3 | 7        | 0.17          |
| (1,387) | 1:A:102:GLY:HA3 | 1:A:102:GLY:H   | 7        | 0.17          |
| (1,379) | 1:A:101:HIS:HB2 | 1:A:101:HIS:H   | 5        | 0.17          |
| (1,360) | 1:A:100:VAL:HA  | 1:A:100:VAL:H   | 2        | 0.17          |
| (1,351) | 1:A:99:GLU:HA   | 1:A:99:GLU:H    | 1        | 0.17          |
| (1,339) | 1:A:98:ILE:HB   | 1:A:98:ILE:H    | 1        | 0.17          |
| (1,339) | 1:A:98:ILE:HB   | 1:A:98:ILE:H    | 4        | 0.17          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG11 | 4        | 0.17          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG12 | 4        | 0.17          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG13 | 4        | 0.17          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG21 | 4        | 0.17          |
| (1,327) | 1:A:97:VAL:HA   | 1:A:97:VAL:HG22 | 4        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG23 | 4        | 0.17          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG11 | 8        | 0.17          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG12 | 8        | 0.17          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG13 | 8        | 0.17          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG21 | 8        | 0.17          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG22 | 8        | 0.17          |
| (1,327)  | 1:A:97:VAL:HA   | 1:A:97:VAL:HG23 | 8        | 0.17          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD11 | 8        | 0.17          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD12 | 8        | 0.17          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD13 | 8        | 0.17          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD21 | 8        | 0.17          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD22 | 8        | 0.17          |
| (1,297)  | 1:A:95:GLY:HA2  | 1:A:94:LEU:HD23 | 8        | 0.17          |
| (1,29)   | 1:A:72:LYS:HB2  | 1:A:72:LYS:H    | 1        | 0.17          |
| (1,29)   | 1:A:72:LYS:HB3  | 1:A:72:LYS:H    | 1        | 0.17          |
| (1,29)   | 1:A:72:LYS:HB2  | 1:A:72:LYS:H    | 5        | 0.17          |
| (1,29)   | 1:A:72:LYS:HB3  | 1:A:72:LYS:H    | 5        | 0.17          |
| (1,28)   | 1:A:72:LYS:H    | 1:A:72:LYS:HA   | 9        | 0.17          |
| (1,267)  | 1:A:90:LYS:HB2  | 1:A:101:HIS:HB3 | 4        | 0.17          |
| (1,267)  | 1:A:90:LYS:HB3  | 1:A:101:HIS:HB3 | 4        | 0.17          |
| (1,260)  | 1:A:89:LEU:HD21 | 1:A:103:LYS:H   | 3        | 0.17          |
| (1,260)  | 1:A:89:LEU:HD22 | 1:A:103:LYS:H   | 3        | 0.17          |
| (1,260)  | 1:A:89:LEU:HD23 | 1:A:103:LYS:H   | 3        | 0.17          |
| (1,260)  | 1:A:89:LEU:HD21 | 1:A:103:LYS:H   | 6        | 0.17          |
| (1,260)  | 1:A:89:LEU:HD22 | 1:A:103:LYS:H   | 6        | 0.17          |
| (1,260)  | 1:A:89:LEU:HD23 | 1:A:103:LYS:H   | 6        | 0.17          |
| (1,250)  | 1:A:89:LEU:HD21 | 1:A:89:LEU:H    | 6        | 0.17          |
| (1,250)  | 1:A:89:LEU:HD22 | 1:A:89:LEU:H    | 6        | 0.17          |
| (1,250)  | 1:A:89:LEU:HD23 | 1:A:89:LEU:H    | 6        | 0.17          |
| (1,195)  | 1:A:84:PHE:HD1  | 1:A:84:PHE:H    | 7        | 0.17          |
| (1,195)  | 1:A:84:PHE:HD2  | 1:A:84:PHE:H    | 7        | 0.17          |
| (1,1752) | 1:A:118:PHE:HA  | 1:B:116:ARG:HA  | 1        | 0.17          |
| (1,175)  | 1:A:83:HIS:HA   | 1:A:83:HIS:HB3  | 7        | 0.17          |
| (1,174)  | 1:A:83:HIS:HA   | 1:A:83:HIS:HB3  | 7        | 0.17          |
| (1,1723) | 1:B:150:LYS:H   | 1:B:149:ARG:H   | 5        | 0.17          |
| (1,1723) | 1:B:150:LYS:H   | 1:B:149:ARG:H   | 9        | 0.17          |
| (1,1721) | 1:B:148:PRO:HB2 | 1:B:149:ARG:H   | 3        | 0.17          |
| (1,1721) | 1:B:148:PRO:HB3 | 1:B:149:ARG:H   | 3        | 0.17          |
| (1,1702) | 1:B:146:ASP:HB2 | 1:B:146:ASP:HA  | 1        | 0.17          |
| (1,1702) | 1:B:146:ASP:HB2 | 1:B:146:ASP:HA  | 5        | 0.17          |
| (1,1699) | 1:B:146:ASP:HB2 | 1:B:146:ASP:HA  | 1        | 0.17          |
| (1,1699) | 1:B:146:ASP:HB2 | 1:B:146:ASP:HA  | 5        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1692) | 1:B:146:ASP:HB2 | 1:B:76:SER:HA   | 3        | 0.17          |
| (1,1691) | 1:B:146:ASP:HB2 | 1:B:76:SER:HA   | 3        | 0.17          |
| (1,1689) | 1:B:145:VAL:HA  | 1:B:146:ASP:H   | 6        | 0.17          |
| (1,168)  | 1:A:81:VAL:HG21 | 1:A:143:LEU:HA  | 6        | 0.17          |
| (1,168)  | 1:A:81:VAL:HG22 | 1:A:143:LEU:HA  | 6        | 0.17          |
| (1,168)  | 1:A:81:VAL:HG23 | 1:A:143:LEU:HA  | 6        | 0.17          |
| (1,1622) | 1:B:138:SER:H   | 1:B:137:LEU:H   | 8        | 0.17          |
| (1,1575) | 1:B:132:THR:H   | 1:B:133:ILE:H   | 4        | 0.17          |
| (1,1573) | 1:B:132:THR:H   | 1:B:133:ILE:H   | 4        | 0.17          |
| (1,157)  | 1:A:81:VAL:HG21 | 1:A:81:VAL:H    | 4        | 0.17          |
| (1,157)  | 1:A:81:VAL:HG22 | 1:A:81:VAL:H    | 4        | 0.17          |
| (1,157)  | 1:A:81:VAL:HG23 | 1:A:81:VAL:H    | 4        | 0.17          |
| (1,1547) | 1:B:128:VAL:H   | 1:B:129:ASP:H   | 3        | 0.17          |
| (1,1547) | 1:B:128:VAL:H   | 1:B:129:ASP:H   | 9        | 0.17          |
| (1,1537) | 1:B:127:ASP:HB3 | 1:B:127:ASP:H   | 5        | 0.17          |
| (1,1537) | 1:B:127:ASP:HB3 | 1:B:127:ASP:H   | 7        | 0.17          |
| (1,1527) | 1:B:126:ALA:HA  | 1:B:128:VAL:H   | 7        | 0.17          |
| (1,1523) | 1:B:125:PRO:HA  | 1:B:127:ASP:H   | 6        | 0.17          |
| (1,1517) | 1:B:125:PRO:HD3 | 1:B:124:ILE:HB  | 4        | 0.17          |
| (1,148)  | 1:A:80:ASP:H    | 1:A:80:ASP:HB3  | 3        | 0.17          |
| (1,148)  | 1:A:80:ASP:H    | 1:A:80:ASP:HB3  | 5        | 0.17          |
| (1,148)  | 1:A:80:ASP:H    | 1:A:80:ASP:HB3  | 9        | 0.17          |
| (1,1473) | 1:B:123:ARG:HB2 | 1:B:123:ARG:HD2 | 5        | 0.17          |
| (1,1473) | 1:B:123:ARG:HB2 | 1:B:123:ARG:HD3 | 5        | 0.17          |
| (1,1473) | 1:B:123:ARG:HB2 | 1:B:123:ARG:HD2 | 9        | 0.17          |
| (1,1473) | 1:B:123:ARG:HB2 | 1:B:123:ARG:HD3 | 9        | 0.17          |
| (1,1460) | 1:B:122:TYR:HB2 | 1:B:122:TYR:HA  | 5        | 0.17          |
| (1,1460) | 1:B:122:TYR:HB3 | 1:B:122:TYR:HA  | 5        | 0.17          |
| (1,1458) | 1:B:122:TYR:HB2 | 1:B:122:TYR:HA  | 5        | 0.17          |
| (1,1458) | 1:B:122:TYR:HB3 | 1:B:122:TYR:HA  | 5        | 0.17          |
| (1,1455) | 1:B:122:TYR:HB2 | 1:B:98:ILE:HD11 | 1        | 0.17          |
| (1,1455) | 1:B:122:TYR:HB2 | 1:B:98:ILE:HD12 | 1        | 0.17          |
| (1,1455) | 1:B:122:TYR:HB2 | 1:B:98:ILE:HD13 | 1        | 0.17          |
| (1,1455) | 1:B:122:TYR:HB3 | 1:B:98:ILE:HD11 | 1        | 0.17          |
| (1,1455) | 1:B:122:TYR:HB3 | 1:B:98:ILE:HD12 | 1        | 0.17          |
| (1,1455) | 1:B:122:TYR:HB3 | 1:B:98:ILE:HD13 | 1        | 0.17          |
| (1,1338) | 1:B:111:HIS:H   | 1:B:112:GLY:H   | 3        | 0.17          |
| (1,1335) | 1:B:111:HIS:H   | 1:B:112:GLY:H   | 3        | 0.17          |
| (1,1321) | 1:B:110:GLU:H   | 1:B:110:GLU:HA  | 3        | 0.17          |
| (1,1321) | 1:B:110:GLU:H   | 1:B:110:GLU:HA  | 9        | 0.17          |
| (1,130)  | 1:A:78:ASN:HB2  | 1:A:79:LEU:H    | 8        | 0.17          |
| (1,1297) | 1:B:107:ARG:H   | 1:B:108:GLN:H   | 1        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1297) | 1:B:107:ARG:H   | 1:B:108:GLN:H   | 5        | 0.17          |
| (1,1285) | 1:B:105:GLU:HG2 | 1:B:115:SER:HB3 | 7        | 0.17          |
| (1,1285) | 1:B:105:GLU:HG3 | 1:B:115:SER:HB3 | 7        | 0.17          |
| (1,1254) | 1:B:102:GLY:HA3 | 1:B:102:GLY:H   | 7        | 0.17          |
| (1,1246) | 1:B:101:HIS:HB2 | 1:B:101:HIS:H   | 5        | 0.17          |
| (1,1227) | 1:B:100:VAL:HA  | 1:B:100:VAL:H   | 2        | 0.17          |
| (1,1218) | 1:B:99:GLU:HA   | 1:B:99:GLU:H    | 1        | 0.17          |
| (1,1206) | 1:B:98:ILE:HB   | 1:B:98:ILE:H    | 1        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG11 | 4        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG12 | 4        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG13 | 4        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG21 | 4        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG22 | 4        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG23 | 4        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG11 | 8        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG12 | 8        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG13 | 8        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG21 | 8        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG22 | 8        | 0.17          |
| (1,1194) | 1:B:97:VAL:HA   | 1:B:97:VAL:HG23 | 8        | 0.17          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD11 | 8        | 0.17          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD12 | 8        | 0.17          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD13 | 8        | 0.17          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD21 | 8        | 0.17          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD22 | 8        | 0.17          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD23 | 8        | 0.17          |
| (1,1115) | 1:A:77:VAL:HG11 | 1:A:145:VAL:H   | 8        | 0.17          |
| (1,1115) | 1:A:77:VAL:HG12 | 1:A:145:VAL:H   | 8        | 0.17          |
| (1,1115) | 1:A:77:VAL:HG13 | 1:A:145:VAL:H   | 8        | 0.17          |
| (1,1134) | 1:B:90:LYS:HB2  | 1:B:101:HIS:HB3 | 4        | 0.17          |
| (1,1134) | 1:B:90:LYS:HB3  | 1:B:101:HIS:HB3 | 4        | 0.17          |
| (1,1127) | 1:B:89:LEU:HD21 | 1:B:103:LYS:H   | 3        | 0.17          |
| (1,1127) | 1:B:89:LEU:HD22 | 1:B:103:LYS:H   | 3        | 0.17          |
| (1,1127) | 1:B:89:LEU:HD23 | 1:B:103:LYS:H   | 3        | 0.17          |
| (1,1112) | 1:A:77:VAL:HG11 | 1:A:122:TYR:HD1 | 7        | 0.17          |
| (1,1112) | 1:A:77:VAL:HG11 | 1:A:122:TYR:HD2 | 7        | 0.17          |
| (1,1112) | 1:A:77:VAL:HG12 | 1:A:122:TYR:HD1 | 7        | 0.17          |
| (1,1112) | 1:A:77:VAL:HG12 | 1:A:122:TYR:HD2 | 7        | 0.17          |
| (1,1112) | 1:A:77:VAL:HG13 | 1:A:122:TYR:HD1 | 7        | 0.17          |
| (1,1112) | 1:A:77:VAL:HG13 | 1:A:122:TYR:HD2 | 7        | 0.17          |
| (1,1117) | 1:B:89:LEU:HD21 | 1:B:89:LEU:H    | 6        | 0.17          |
| (1,1117) | 1:B:89:LEU:HD22 | 1:B:89:LEU:H    | 6        | 0.17          |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (1,1117) | 1:B:89:LEU:HD23  | 1:B:89:LEU:H   | 6        | 0.17          |
| (1,1062) | 1:B:84:PHE:HD1   | 1:B:84:PHE:H   | 7        | 0.17          |
| (1,1062) | 1:B:84:PHE:HD2   | 1:B:84:PHE:H   | 7        | 0.17          |
| (1,1045) | 1:B:83:HIS:HB3   | 1:B:83:HIS:H   | 6        | 0.17          |
| (1,1042) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3 | 7        | 0.17          |
| (1,1041) | 1:B:83:HIS:HA    | 1:B:83:HIS:HB3 | 7        | 0.17          |
| (1,1035) | 1:B:81:VAL:HG21  | 1:B:143:LEU:HA | 6        | 0.17          |
| (1,1035) | 1:B:81:VAL:HG22  | 1:B:143:LEU:HA | 6        | 0.17          |
| (1,1035) | 1:B:81:VAL:HG23  | 1:B:143:LEU:HA | 6        | 0.17          |
| (1,103)  | 1:A:77:VAL:H     | 1:A:78:ASN:H   | 4        | 0.17          |
| (1,1015) | 1:B:80:ASP:H     | 1:B:80:ASP:HB3 | 3        | 0.17          |
| (1,1015) | 1:B:80:ASP:H     | 1:B:80:ASP:HB3 | 5        | 0.17          |
| (1,1015) | 1:B:80:ASP:H     | 1:B:80:ASP:HB3 | 9        | 0.17          |
| (1,982)  | 1:B:77:VAL:HG11  | 1:B:145:VAL:H  | 3        | 0.16          |
| (1,982)  | 1:B:77:VAL:HG12  | 1:B:145:VAL:H  | 3        | 0.16          |
| (1,982)  | 1:B:77:VAL:HG13  | 1:B:145:VAL:H  | 3        | 0.16          |
| (1,982)  | 1:B:77:VAL:HG11  | 1:B:145:VAL:H  | 4        | 0.16          |
| (1,982)  | 1:B:77:VAL:HG12  | 1:B:145:VAL:H  | 4        | 0.16          |
| (1,982)  | 1:B:77:VAL:HG13  | 1:B:145:VAL:H  | 4        | 0.16          |
| (1,970)  | 1:B:77:VAL:H     | 1:B:78:ASN:H   | 7        | 0.16          |
| (1,947)  | 1:B:77:VAL:HA    | 1:B:68:MET:HA  | 5        | 0.16          |
| (1,896)  | 1:B:72:LYS:HB2   | 1:B:72:LYS:H   | 9        | 0.16          |
| (1,896)  | 1:B:72:LYS:HB3   | 1:B:72:LYS:H   | 9        | 0.16          |
| (1,856)  | 1:A:150:LYS:H    | 1:A:149:ARG:H  | 2        | 0.16          |
| (1,835)  | 1:A:146:ASP:HB2  | 1:A:146:ASP:HA | 3        | 0.16          |
| (1,832)  | 1:A:146:ASP:HB2  | 1:A:146:ASP:HA | 3        | 0.16          |
| (1,827)  | 1:A:146:ASP:HB3  | 1:A:76:SER:HA  | 2        | 0.16          |
| (1,826)  | 1:A:146:ASP:HB3  | 1:A:76:SER:HA  | 2        | 0.16          |
| (1,825)  | 1:A:146:ASP:HB2  | 1:A:76:SER:HA  | 3        | 0.16          |
| (1,824)  | 1:A:146:ASP:HB2  | 1:A:76:SER:HA  | 3        | 0.16          |
| (1,808)  | 1:A:144:THR:H    | 1:A:145:VAL:H  | 4        | 0.16          |
| (1,803)  | 1:A:144:THR:H    | 1:A:145:VAL:H  | 4        | 0.16          |
| (1,80)   | 1:A:77:VAL:HA    | 1:A:68:MET:HA  | 5        | 0.16          |
| (1,785)  | 1:A:142:VAL:HG11 | 1:A:143:LEU:H  | 2        | 0.16          |
| (1,785)  | 1:A:142:VAL:HG12 | 1:A:143:LEU:H  | 2        | 0.16          |
| (1,785)  | 1:A:142:VAL:HG13 | 1:A:143:LEU:H  | 2        | 0.16          |
| (1,785)  | 1:A:142:VAL:HG21 | 1:A:143:LEU:H  | 2        | 0.16          |
| (1,785)  | 1:A:142:VAL:HG22 | 1:A:143:LEU:H  | 2        | 0.16          |
| (1,785)  | 1:A:142:VAL:HG23 | 1:A:143:LEU:H  | 2        | 0.16          |
| (1,755)  | 1:A:138:SER:H    | 1:A:137:LEU:H  | 2        | 0.16          |
| (1,755)  | 1:A:138:SER:H    | 1:A:137:LEU:H  | 8        | 0.16          |
| (1,675)  | 1:A:128:VAL:H    | 1:A:126:ALA:H  | 6        | 0.16          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,593) | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA  | 4        | 0.16          |
| (1,593) | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA  | 4        | 0.16          |
| (1,591) | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA  | 4        | 0.16          |
| (1,591) | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA  | 4        | 0.16          |
| (1,551) | 1:A:118:PHE:HD1  | 1:A:103:LYS:HA  | 4        | 0.16          |
| (1,551) | 1:A:118:PHE:HD2  | 1:A:103:LYS:HA  | 4        | 0.16          |
| (1,471) | 1:A:111:HIS:H    | 1:A:112:GLY:H   | 9        | 0.16          |
| (1,468) | 1:A:111:HIS:H    | 1:A:112:GLY:H   | 9        | 0.16          |
| (1,437) | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD1 | 7        | 0.16          |
| (1,437) | 1:A:107:ARG:HB2  | 1:A:113:PHE:HD2 | 7        | 0.16          |
| (1,424) | 1:A:107:ARG:HG2  | 1:A:107:ARG:HA  | 5        | 0.16          |
| (1,424) | 1:A:107:ARG:HG3  | 1:A:107:ARG:HA  | 5        | 0.16          |
| (1,417) | 1:A:105:GLU:HG2  | 1:A:106:GLU:H   | 2        | 0.16          |
| (1,417) | 1:A:105:GLU:HG3  | 1:A:106:GLU:H   | 2        | 0.16          |
| (1,358) | 1:A:100:VAL:HG11 | 1:A:92:LYS:H    | 3        | 0.16          |
| (1,358) | 1:A:100:VAL:HG12 | 1:A:92:LYS:H    | 3        | 0.16          |
| (1,358) | 1:A:100:VAL:HG13 | 1:A:92:LYS:H    | 3        | 0.16          |
| (1,358) | 1:A:100:VAL:HG11 | 1:A:92:LYS:H    | 4        | 0.16          |
| (1,358) | 1:A:100:VAL:HG12 | 1:A:92:LYS:H    | 4        | 0.16          |
| (1,358) | 1:A:100:VAL:HG13 | 1:A:92:LYS:H    | 4        | 0.16          |
| (1,341) | 1:A:98:ILE:HB    | 1:A:99:GLU:H    | 6        | 0.16          |
| (1,335) | 1:A:98:ILE:H     | 1:A:97:VAL:H    | 2        | 0.16          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG11 | 5        | 0.16          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG12 | 5        | 0.16          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG13 | 5        | 0.16          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG21 | 5        | 0.16          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG22 | 5        | 0.16          |
| (1,327) | 1:A:97:VAL:HA    | 1:A:97:VAL:HG23 | 5        | 0.16          |
| (1,282) | 1:A:93:VAL:H     | 1:A:92:LYS:HG2  | 1        | 0.16          |
| (1,282) | 1:A:93:VAL:H     | 1:A:92:LYS:HG3  | 1        | 0.16          |
| (1,260) | 1:A:89:LEU:HD21  | 1:A:103:LYS:H   | 8        | 0.16          |
| (1,260) | 1:A:89:LEU:HD22  | 1:A:103:LYS:H   | 8        | 0.16          |
| (1,260) | 1:A:89:LEU:HD23  | 1:A:103:LYS:H   | 8        | 0.16          |
| (1,250) | 1:A:89:LEU:HD21  | 1:A:89:LEU:H    | 8        | 0.16          |
| (1,250) | 1:A:89:LEU:HD22  | 1:A:89:LEU:H    | 8        | 0.16          |
| (1,250) | 1:A:89:LEU:HD23  | 1:A:89:LEU:H    | 8        | 0.16          |
| (1,236) | 1:A:89:LEU:HD21  | 1:A:85:SER:HB3  | 5        | 0.16          |
| (1,236) | 1:A:89:LEU:HD22  | 1:A:85:SER:HB3  | 5        | 0.16          |
| (1,236) | 1:A:89:LEU:HD23  | 1:A:85:SER:HB3  | 5        | 0.16          |
| (1,216) | 1:A:85:SER:HB2   | 1:A:89:LEU:H    | 5        | 0.16          |
| (1,215) | 1:A:85:SER:HB3   | 1:A:89:LEU:H    | 9        | 0.16          |
| (1,203) | 1:A:84:PHE:HE1   | 1:A:116:ARG:H   | 8        | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,203)  | 1:A:84:PHE:HE2  | 1:A:116:ARG:H    | 8        | 0.16          |
| (1,195)  | 1:A:84:PHE:HD1  | 1:A:84:PHE:H     | 4        | 0.16          |
| (1,195)  | 1:A:84:PHE:HD2  | 1:A:84:PHE:H     | 4        | 0.16          |
| (1,193)  | 1:A:84:PHE:HD1  | 1:A:83:HIS:HA    | 4        | 0.16          |
| (1,193)  | 1:A:84:PHE:HD2  | 1:A:83:HIS:HA    | 4        | 0.16          |
| (1,178)  | 1:A:83:HIS:HB3  | 1:A:83:HIS:H     | 6        | 0.16          |
| (1,1770) | 1:A:123:ARG:HD2 | 1:B:113:PHE:H    | 3        | 0.16          |
| (1,1770) | 1:A:123:ARG:HD3 | 1:B:113:PHE:H    | 3        | 0.16          |
| (1,1723) | 1:B:150:LYS:H   | 1:B:149:ARG:H    | 2        | 0.16          |
| (1,1702) | 1:B:146:ASP:HB2 | 1:B:146:ASP:HA   | 3        | 0.16          |
| (1,1699) | 1:B:146:ASP:HB2 | 1:B:146:ASP:HA   | 3        | 0.16          |
| (1,1694) | 1:B:146:ASP:HB3 | 1:B:76:SER:HA    | 2        | 0.16          |
| (1,1693) | 1:B:146:ASP:HB3 | 1:B:76:SER:HA    | 2        | 0.16          |
| (1,1684) | 1:B:145:VAL:HB  | 1:B:145:VAL:H    | 4        | 0.16          |
| (1,1675) | 1:B:144:THR:H   | 1:B:145:VAL:H    | 4        | 0.16          |
| (1,1670) | 1:B:144:THR:H   | 1:B:145:VAL:H    | 4        | 0.16          |
| (1,167)  | 1:A:81:VAL:H    | 1:A:141:GLY:HA2  | 7        | 0.16          |
| (1,1622) | 1:B:138:SER:H   | 1:B:137:LEU:H    | 2        | 0.16          |
| (1,1605) | 1:B:135:SER:HA  | 1:B:145:VAL:HG21 | 3        | 0.16          |
| (1,1605) | 1:B:135:SER:HA  | 1:B:145:VAL:HG22 | 3        | 0.16          |
| (1,1605) | 1:B:135:SER:HA  | 1:B:145:VAL:HG23 | 3        | 0.16          |
| (1,160)  | 1:A:81:VAL:H    | 1:A:82:LYS:H     | 9        | 0.16          |
| (1,159)  | 1:A:81:VAL:H    | 1:A:82:LYS:H     | 9        | 0.16          |
| (1,1542) | 1:B:128:VAL:H   | 1:B:126:ALA:H    | 6        | 0.16          |
| (1,148)  | 1:A:80:ASP:H    | 1:A:80:ASP:HB3   | 2        | 0.16          |
| (1,148)  | 1:A:80:ASP:H    | 1:A:80:ASP:HB3   | 4        | 0.16          |
| (1,148)  | 1:A:80:ASP:H    | 1:A:80:ASP:HB3   | 8        | 0.16          |
| (1,1460) | 1:B:122:TYR:HB2 | 1:B:122:TYR:HA   | 4        | 0.16          |
| (1,1460) | 1:B:122:TYR:HB3 | 1:B:122:TYR:HA   | 4        | 0.16          |
| (1,1458) | 1:B:122:TYR:HB2 | 1:B:122:TYR:HA   | 4        | 0.16          |
| (1,1458) | 1:B:122:TYR:HB3 | 1:B:122:TYR:HA   | 4        | 0.16          |
| (1,1443) | 1:B:119:HIS:HB3 | 1:B:119:HIS:HA   | 1        | 0.16          |
| (1,1442) | 1:B:119:HIS:HB3 | 1:B:119:HIS:HA   | 1        | 0.16          |
| (1,1418) | 1:B:118:PHE:HD1 | 1:B:103:LYS:HA   | 4        | 0.16          |
| (1,1418) | 1:B:118:PHE:HD2 | 1:B:103:LYS:HA   | 4        | 0.16          |
| (1,1338) | 1:B:111:HIS:H   | 1:B:112:GLY:H    | 9        | 0.16          |
| (1,1335) | 1:B:111:HIS:H   | 1:B:112:GLY:H    | 9        | 0.16          |
| (1,1321) | 1:B:110:GLU:H   | 1:B:110:GLU:HA   | 7        | 0.16          |
| (1,1304) | 1:B:107:ARG:HB2 | 1:B:113:PHE:HD1  | 7        | 0.16          |
| (1,1304) | 1:B:107:ARG:HB2 | 1:B:113:PHE:HD2  | 7        | 0.16          |
| (1,130)  | 1:A:78:ASN:HB2  | 1:A:79:LEU:H     | 9        | 0.16          |
| (1,1284) | 1:B:105:GLU:HG2 | 1:B:106:GLU:H    | 2        | 0.16          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1284) | 1:B:105:GLU:HG3  | 1:B:106:GLU:H   | 2        | 0.16          |
| (1,1225) | 1:B:100:VAL:HG11 | 1:B:92:LYS:H    | 3        | 0.16          |
| (1,1225) | 1:B:100:VAL:HG12 | 1:B:92:LYS:H    | 3        | 0.16          |
| (1,1225) | 1:B:100:VAL:HG13 | 1:B:92:LYS:H    | 3        | 0.16          |
| (1,1225) | 1:B:100:VAL:HG11 | 1:B:92:LYS:H    | 4        | 0.16          |
| (1,1225) | 1:B:100:VAL:HG12 | 1:B:92:LYS:H    | 4        | 0.16          |
| (1,1225) | 1:B:100:VAL:HG13 | 1:B:92:LYS:H    | 4        | 0.16          |
| (1,1208) | 1:B:98:ILE:HB    | 1:B:99:GLU:H    | 6        | 0.16          |
| (1,1202) | 1:B:98:ILE:H     | 1:B:97:VAL:H    | 2        | 0.16          |
| (1,1194) | 1:B:97:VAL:HA    | 1:B:97:VAL:HG11 | 5        | 0.16          |
| (1,1194) | 1:B:97:VAL:HA    | 1:B:97:VAL:HG12 | 5        | 0.16          |
| (1,1194) | 1:B:97:VAL:HA    | 1:B:97:VAL:HG13 | 5        | 0.16          |
| (1,1194) | 1:B:97:VAL:HA    | 1:B:97:VAL:HG21 | 5        | 0.16          |
| (1,1194) | 1:B:97:VAL:HA    | 1:B:97:VAL:HG22 | 5        | 0.16          |
| (1,1194) | 1:B:97:VAL:HA    | 1:B:97:VAL:HG23 | 5        | 0.16          |
| (1,115)  | 1:A:77:VAL:HG11  | 1:A:145:VAL:H   | 3        | 0.16          |
| (1,115)  | 1:A:77:VAL:HG12  | 1:A:145:VAL:H   | 3        | 0.16          |
| (1,115)  | 1:A:77:VAL:HG13  | 1:A:145:VAL:H   | 3        | 0.16          |
| (1,115)  | 1:A:77:VAL:HG11  | 1:A:145:VAL:H   | 4        | 0.16          |
| (1,115)  | 1:A:77:VAL:HG12  | 1:A:145:VAL:H   | 4        | 0.16          |
| (1,115)  | 1:A:77:VAL:HG13  | 1:A:145:VAL:H   | 4        | 0.16          |
| (1,1149) | 1:B:93:VAL:H     | 1:B:92:LYS:HG2  | 1        | 0.16          |
| (1,1149) | 1:B:93:VAL:H     | 1:B:92:LYS:HG3  | 1        | 0.16          |
| (1,1127) | 1:B:89:LEU:HD21  | 1:B:103:LYS:H   | 6        | 0.16          |
| (1,1127) | 1:B:89:LEU:HD22  | 1:B:103:LYS:H   | 6        | 0.16          |
| (1,1127) | 1:B:89:LEU:HD23  | 1:B:103:LYS:H   | 6        | 0.16          |
| (1,1127) | 1:B:89:LEU:HD21  | 1:B:103:LYS:H   | 8        | 0.16          |
| (1,1127) | 1:B:89:LEU:HD22  | 1:B:103:LYS:H   | 8        | 0.16          |
| (1,1127) | 1:B:89:LEU:HD23  | 1:B:103:LYS:H   | 8        | 0.16          |
| (1,1117) | 1:B:89:LEU:HD21  | 1:B:89:LEU:H    | 8        | 0.16          |
| (1,1117) | 1:B:89:LEU:HD22  | 1:B:89:LEU:H    | 8        | 0.16          |
| (1,1117) | 1:B:89:LEU:HD23  | 1:B:89:LEU:H    | 8        | 0.16          |
| (1,1083) | 1:B:85:SER:HB2   | 1:B:89:LEU:H    | 5        | 0.16          |
| (1,1082) | 1:B:85:SER:HB3   | 1:B:89:LEU:H    | 9        | 0.16          |
| (1,1070) | 1:B:84:PHE:HE1   | 1:B:116:ARG:H   | 8        | 0.16          |
| (1,1070) | 1:B:84:PHE:HE2   | 1:B:116:ARG:H   | 8        | 0.16          |
| (1,1062) | 1:B:84:PHE:HD1   | 1:B:84:PHE:H    | 4        | 0.16          |
| (1,1062) | 1:B:84:PHE:HD2   | 1:B:84:PHE:H    | 4        | 0.16          |
| (1,1060) | 1:B:84:PHE:HD1   | 1:B:83:HIS:HA   | 4        | 0.16          |
| (1,1060) | 1:B:84:PHE:HD2   | 1:B:83:HIS:HA   | 4        | 0.16          |
| (1,1034) | 1:B:81:VAL:H     | 1:B:141:GLY:HA2 | 7        | 0.16          |
| (1,103)  | 1:A:77:VAL:H     | 1:A:78:ASN:H    | 7        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1027) | 1:B:81:VAL:H     | 1:B:82:LYS:H     | 9        | 0.16          |
| (1,1026) | 1:B:81:VAL:H     | 1:B:82:LYS:H     | 9        | 0.16          |
| (1,1015) | 1:B:80:ASP:H     | 1:B:80:ASP:HB3   | 2        | 0.16          |
| (1,1015) | 1:B:80:ASP:H     | 1:B:80:ASP:HB3   | 4        | 0.16          |
| (1,1015) | 1:B:80:ASP:H     | 1:B:80:ASP:HB3   | 8        | 0.16          |
| (1,997)  | 1:B:78:ASN:HB2   | 1:B:79:LEU:H     | 9        | 0.15          |
| (1,978)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HE1  | 8        | 0.15          |
| (1,978)  | 1:B:77:VAL:HG11  | 1:B:122:TYR:HE2  | 8        | 0.15          |
| (1,978)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HE1  | 8        | 0.15          |
| (1,978)  | 1:B:77:VAL:HG12  | 1:B:122:TYR:HE2  | 8        | 0.15          |
| (1,978)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HE1  | 8        | 0.15          |
| (1,978)  | 1:B:77:VAL:HG13  | 1:B:122:TYR:HE2  | 8        | 0.15          |
| (1,970)  | 1:B:77:VAL:H     | 1:B:78:ASN:H     | 1        | 0.15          |
| (1,970)  | 1:B:77:VAL:H     | 1:B:78:ASN:H     | 3        | 0.15          |
| (1,969)  | 1:B:77:VAL:HG11  | 1:B:78:ASN:H     | 3        | 0.15          |
| (1,969)  | 1:B:77:VAL:HG12  | 1:B:78:ASN:H     | 3        | 0.15          |
| (1,969)  | 1:B:77:VAL:HG13  | 1:B:78:ASN:H     | 3        | 0.15          |
| (1,942)  | 1:B:76:SER:HB3   | 1:B:146:ASP:HB3  | 6        | 0.15          |
| (1,939)  | 1:B:76:SER:HB3   | 1:B:146:ASP:HB2  | 5        | 0.15          |
| (1,938)  | 1:B:76:SER:HB3   | 1:B:146:ASP:HB2  | 5        | 0.15          |
| (1,926)  | 1:B:76:SER:HB2   | 1:B:75:PHE:HD1   | 5        | 0.15          |
| (1,926)  | 1:B:76:SER:HB2   | 1:B:75:PHE:HD2   | 5        | 0.15          |
| (1,914)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HD1   | 7        | 0.15          |
| (1,914)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HD2   | 7        | 0.15          |
| (1,896)  | 1:B:72:LYS:HB2   | 1:B:72:LYS:H     | 7        | 0.15          |
| (1,896)  | 1:B:72:LYS:HB3   | 1:B:72:LYS:H     | 7        | 0.15          |
| (1,895)  | 1:B:72:LYS:H     | 1:B:72:LYS:HA    | 1        | 0.15          |
| (1,894)  | 1:B:72:LYS:H     | 1:B:71:GLU:HA    | 7        | 0.15          |
| (1,893)  | 1:B:71:GLU:H     | 1:B:76:SER:H     | 5        | 0.15          |
| (1,874)  | 1:B:68:MET:HA    | 1:B:68:MET:HG2   | 4        | 0.15          |
| (1,874)  | 1:B:68:MET:HA    | 1:B:68:MET:HG3   | 4        | 0.15          |
| (1,874)  | 1:B:68:MET:HA    | 1:B:68:MET:HG2   | 6        | 0.15          |
| (1,874)  | 1:B:68:MET:HA    | 1:B:68:MET:HG3   | 6        | 0.15          |
| (1,866)  | 1:A:152:VAL:H    | 1:A:151:GLN:H    | 9        | 0.15          |
| (1,842)  | 1:A:147:GLY:HA3  | 1:A:133:ILE:HB   | 8        | 0.15          |
| (1,809)  | 1:A:144:THR:HG21 | 1:A:146:ASP:HB3  | 4        | 0.15          |
| (1,809)  | 1:A:144:THR:HG22 | 1:A:146:ASP:HB3  | 4        | 0.15          |
| (1,809)  | 1:A:144:THR:HG23 | 1:A:146:ASP:HB3  | 4        | 0.15          |
| (1,778)  | 1:A:142:VAL:H    | 1:A:141:GLY:H    | 5        | 0.15          |
| (1,777)  | 1:A:142:VAL:H    | 1:A:141:GLY:H    | 5        | 0.15          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD11 | 5        | 0.15          |
| (1,750)  | 1:A:136:SER:H    | 1:A:143:LEU:HD12 | 5        | 0.15          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,750) | 1:A:136:SER:H    | 1:A:143:LEU:HD13 | 5        | 0.15          |
| (1,750) | 1:A:136:SER:H    | 1:A:143:LEU:HD21 | 5        | 0.15          |
| (1,750) | 1:A:136:SER:H    | 1:A:143:LEU:HD22 | 5        | 0.15          |
| (1,750) | 1:A:136:SER:H    | 1:A:143:LEU:HD23 | 5        | 0.15          |
| (1,75)  | 1:A:76:SER:HB3   | 1:A:146:ASP:HB3  | 6        | 0.15          |
| (1,749) | 1:A:136:SER:HA   | 1:A:137:LEU:H    | 2        | 0.15          |
| (1,749) | 1:A:136:SER:HA   | 1:A:137:LEU:H    | 7        | 0.15          |
| (1,746) | 1:A:136:SER:H    | 1:A:135:SER:H    | 4        | 0.15          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG21 | 3        | 0.15          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG22 | 3        | 0.15          |
| (1,738) | 1:A:135:SER:HA   | 1:A:145:VAL:HG23 | 3        | 0.15          |
| (1,737) | 1:A:135:SER:HA   | 1:A:136:SER:H    | 8        | 0.15          |
| (1,72)  | 1:A:76:SER:HB3   | 1:A:146:ASP:HB2  | 5        | 0.15          |
| (1,71)  | 1:A:76:SER:HB3   | 1:A:146:ASP:HB2  | 5        | 0.15          |
| (1,7)   | 1:A:68:MET:HA    | 1:A:68:MET:HG2   | 4        | 0.15          |
| (1,7)   | 1:A:68:MET:HA    | 1:A:68:MET:HG3   | 4        | 0.15          |
| (1,7)   | 1:A:68:MET:HA    | 1:A:68:MET:HG2   | 6        | 0.15          |
| (1,7)   | 1:A:68:MET:HA    | 1:A:68:MET:HG3   | 6        | 0.15          |
| (1,681) | 1:A:128:VAL:H    | 1:A:150:LYS:HD2  | 9        | 0.15          |
| (1,681) | 1:A:128:VAL:H    | 1:A:150:LYS:HD3  | 9        | 0.15          |
| (1,615) | 1:A:124:ILE:HB   | 1:A:97:VAL:HA    | 5        | 0.15          |
| (1,614) | 1:A:124:ILE:HD11 | 1:A:96:ASP:H     | 9        | 0.15          |
| (1,614) | 1:A:124:ILE:HD12 | 1:A:96:ASP:H     | 9        | 0.15          |
| (1,614) | 1:A:124:ILE:HD13 | 1:A:96:ASP:H     | 9        | 0.15          |
| (1,596) | 1:A:122:TYR:HA   | 1:A:122:TYR:H    | 9        | 0.15          |
| (1,593) | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA   | 7        | 0.15          |
| (1,593) | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA   | 7        | 0.15          |
| (1,591) | 1:A:122:TYR:HB2  | 1:A:122:TYR:HA   | 7        | 0.15          |
| (1,591) | 1:A:122:TYR:HB3  | 1:A:122:TYR:HA   | 7        | 0.15          |
| (1,59)  | 1:A:76:SER:HB2   | 1:A:75:PHE:HD1   | 5        | 0.15          |
| (1,59)  | 1:A:76:SER:HB2   | 1:A:75:PHE:HD2   | 5        | 0.15          |
| (1,576) | 1:A:119:HIS:HB3  | 1:A:119:HIS:HA   | 1        | 0.15          |
| (1,575) | 1:A:119:HIS:HB3  | 1:A:119:HIS:HA   | 1        | 0.15          |
| (1,542) | 1:A:117:GLU:HA   | 1:A:103:LYS:HD2  | 9        | 0.15          |
| (1,542) | 1:A:117:GLU:HA   | 1:A:103:LYS:HD3  | 9        | 0.15          |
| (1,533) | 1:A:115:SER:HB2  | 1:A:116:ARG:H    | 3        | 0.15          |
| (1,521) | 1:A:115:SER:HB2  | 1:A:105:GLU:HB2  | 1        | 0.15          |
| (1,521) | 1:A:115:SER:HB2  | 1:A:105:GLU:HB3  | 1        | 0.15          |
| (1,485) | 1:A:113:PHE:HA   | 1:A:108:GLN:HA   | 1        | 0.15          |
| (1,478) | 1:A:112:GLY:HA2  | 1:A:112:GLY:H    | 7        | 0.15          |
| (1,47)  | 1:A:75:PHE:HA    | 1:A:75:PHE:HD1   | 7        | 0.15          |
| (1,47)  | 1:A:75:PHE:HA    | 1:A:75:PHE:HD2   | 7        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,442)  | 1:A:108:GLN:HA  | 1:A:108:GLN:HB2 | 2        | 0.15          |
| (1,442)  | 1:A:108:GLN:HA  | 1:A:108:GLN:HB3 | 2        | 0.15          |
| (1,438)  | 1:A:107:ARG:HB3 | 1:A:113:PHE:HD1 | 3        | 0.15          |
| (1,438)  | 1:A:107:ARG:HB3 | 1:A:113:PHE:HD2 | 3        | 0.15          |
| (1,415)  | 1:A:105:GLU:HA  | 1:A:106:GLU:H   | 9        | 0.15          |
| (1,395)  | 1:A:103:LYS:HG2 | 1:A:103:LYS:H   | 8        | 0.15          |
| (1,395)  | 1:A:103:LYS:HG3 | 1:A:103:LYS:H   | 8        | 0.15          |
| (1,379)  | 1:A:101:HIS:HB2 | 1:A:101:HIS:H   | 6        | 0.15          |
| (1,367)  | 1:A:101:HIS:HB3 | 1:A:92:LYS:HB2  | 3        | 0.15          |
| (1,367)  | 1:A:101:HIS:HB3 | 1:A:92:LYS:HB3  | 3        | 0.15          |
| (1,362)  | 1:A:100:VAL:H   | 1:A:100:VAL:HB  | 5        | 0.15          |
| (1,360)  | 1:A:100:VAL:HA  | 1:A:100:VAL:H   | 8        | 0.15          |
| (1,341)  | 1:A:98:ILE:HB   | 1:A:99:GLU:H    | 2        | 0.15          |
| (1,339)  | 1:A:98:ILE:HB   | 1:A:98:ILE:H    | 7        | 0.15          |
| (1,339)  | 1:A:98:ILE:HB   | 1:A:98:ILE:H    | 9        | 0.15          |
| (1,335)  | 1:A:98:ILE:H    | 1:A:97:VAL:H    | 9        | 0.15          |
| (1,326)  | 1:A:97:VAL:HB   | 1:A:97:VAL:HA   | 3        | 0.15          |
| (1,326)  | 1:A:97:VAL:HB   | 1:A:97:VAL:HA   | 5        | 0.15          |
| (1,325)  | 1:A:97:VAL:HB   | 1:A:97:VAL:HA   | 3        | 0.15          |
| (1,325)  | 1:A:97:VAL:HB   | 1:A:97:VAL:HA   | 5        | 0.15          |
| (1,293)  | 1:A:94:LEU:H    | 1:A:95:GLY:H    | 5        | 0.15          |
| (1,29)   | 1:A:72:LYS:HB2  | 1:A:72:LYS:H    | 7        | 0.15          |
| (1,29)   | 1:A:72:LYS:HB3  | 1:A:72:LYS:H    | 7        | 0.15          |
| (1,29)   | 1:A:72:LYS:HB2  | 1:A:72:LYS:H    | 9        | 0.15          |
| (1,29)   | 1:A:72:LYS:HB3  | 1:A:72:LYS:H    | 9        | 0.15          |
| (1,28)   | 1:A:72:LYS:H    | 1:A:72:LYS:HA   | 1        | 0.15          |
| (1,275)  | 1:A:92:LYS:H    | 1:A:92:LYS:HG2  | 2        | 0.15          |
| (1,275)  | 1:A:92:LYS:H    | 1:A:92:LYS:HG3  | 2        | 0.15          |
| (1,27)   | 1:A:72:LYS:H    | 1:A:71:GLU:HA   | 7        | 0.15          |
| (1,26)   | 1:A:71:GLU:H    | 1:A:76:SER:H    | 5        | 0.15          |
| (1,242)  | 1:A:89:LEU:H    | 1:A:88:GLU:H    | 8        | 0.15          |
| (1,241)  | 1:A:89:LEU:H    | 1:A:88:GLU:H    | 8        | 0.15          |
| (1,239)  | 1:A:89:LEU:H    | 1:A:87:GLU:HA   | 3        | 0.15          |
| (1,235)  | 1:A:88:GLU:H    | 1:A:89:LEU:HB2  | 5        | 0.15          |
| (1,235)  | 1:A:88:GLU:H    | 1:A:89:LEU:HB3  | 5        | 0.15          |
| (1,231)  | 1:A:87:GLU:HB2  | 1:A:89:LEU:H    | 1        | 0.15          |
| (1,231)  | 1:A:87:GLU:HB3  | 1:A:89:LEU:H    | 1        | 0.15          |
| (1,186)  | 1:A:83:HIS:HB2  | 1:A:104:HIS:HB2 | 4        | 0.15          |
| (1,178)  | 1:A:83:HIS:HB3  | 1:A:83:HIS:H    | 8        | 0.15          |
| (1,1755) | 1:A:118:PHE:HD1 | 1:B:116:ARG:HA  | 4        | 0.15          |
| (1,1755) | 1:A:118:PHE:HD2 | 1:B:116:ARG:HA  | 4        | 0.15          |
| (1,1733) | 1:B:152:VAL:H   | 1:B:151:GLN:H   | 9        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1709) | 1:B:147:GLY:HA3  | 1:B:133:ILE:HB   | 8        | 0.15          |
| (1,1652) | 1:B:142:VAL:HG11 | 1:B:143:LEU:H    | 2        | 0.15          |
| (1,1652) | 1:B:142:VAL:HG12 | 1:B:143:LEU:H    | 2        | 0.15          |
| (1,1652) | 1:B:142:VAL:HG13 | 1:B:143:LEU:H    | 2        | 0.15          |
| (1,1652) | 1:B:142:VAL:HG21 | 1:B:143:LEU:H    | 2        | 0.15          |
| (1,1652) | 1:B:142:VAL:HG22 | 1:B:143:LEU:H    | 2        | 0.15          |
| (1,1652) | 1:B:142:VAL:HG23 | 1:B:143:LEU:H    | 2        | 0.15          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD11 | 5        | 0.15          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD12 | 5        | 0.15          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD13 | 5        | 0.15          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD21 | 5        | 0.15          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD22 | 5        | 0.15          |
| (1,1617) | 1:B:136:SER:H    | 1:B:143:LEU:HD23 | 5        | 0.15          |
| (1,1616) | 1:B:136:SER:HA   | 1:B:137:LEU:H    | 2        | 0.15          |
| (1,1616) | 1:B:136:SER:HA   | 1:B:137:LEU:H    | 7        | 0.15          |
| (1,1613) | 1:B:136:SER:H    | 1:B:135:SER:H    | 4        | 0.15          |
| (1,1604) | 1:B:135:SER:HA   | 1:B:136:SER:H    | 8        | 0.15          |
| (1,1567) | 1:B:132:THR:HG21 | 1:B:132:THR:H    | 4        | 0.15          |
| (1,1567) | 1:B:132:THR:HG22 | 1:B:132:THR:H    | 4        | 0.15          |
| (1,1567) | 1:B:132:THR:HG23 | 1:B:132:THR:H    | 4        | 0.15          |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD2  | 9        | 0.15          |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD3  | 9        | 0.15          |
| (1,1482) | 1:B:124:ILE:HB   | 1:B:97:VAL:HA    | 5        | 0.15          |
| (1,1481) | 1:B:124:ILE:HD11 | 1:B:96:ASP:H     | 9        | 0.15          |
| (1,1481) | 1:B:124:ILE:HD12 | 1:B:96:ASP:H     | 9        | 0.15          |
| (1,1481) | 1:B:124:ILE:HD13 | 1:B:96:ASP:H     | 9        | 0.15          |
| (1,1463) | 1:B:122:TYR:HA   | 1:B:122:TYR:H    | 9        | 0.15          |
| (1,1460) | 1:B:122:TYR:HB2  | 1:B:122:TYR:HA   | 7        | 0.15          |
| (1,1460) | 1:B:122:TYR:HB3  | 1:B:122:TYR:HA   | 7        | 0.15          |
| (1,1458) | 1:B:122:TYR:HB2  | 1:B:122:TYR:HA   | 7        | 0.15          |
| (1,1458) | 1:B:122:TYR:HB3  | 1:B:122:TYR:HA   | 7        | 0.15          |
| (1,1409) | 1:B:117:GLU:HA   | 1:B:103:LYS:HD2  | 9        | 0.15          |
| (1,1409) | 1:B:117:GLU:HA   | 1:B:103:LYS:HD3  | 9        | 0.15          |
| (1,1400) | 1:B:115:SER:HB2  | 1:B:116:ARG:H    | 3        | 0.15          |
| (1,1388) | 1:B:115:SER:HB2  | 1:B:105:GLU:HB2  | 1        | 0.15          |
| (1,1388) | 1:B:115:SER:HB2  | 1:B:105:GLU:HB3  | 1        | 0.15          |
| (1,1352) | 1:B:113:PHE:HA   | 1:B:108:GLN:HA   | 1        | 0.15          |
| (1,1345) | 1:B:112:GLY:HA2  | 1:B:112:GLY:H    | 7        | 0.15          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB2  | 2        | 0.15          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB3  | 2        | 0.15          |
| (1,1305) | 1:B:107:ARG:HB3  | 1:B:113:PHE:HD1  | 3        | 0.15          |
| (1,1305) | 1:B:107:ARG:HB3  | 1:B:113:PHE:HD2  | 3        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1291) | 1:B:107:ARG:HG2 | 1:B:107:ARG:HA  | 5        | 0.15          |
| (1,1291) | 1:B:107:ARG:HG3 | 1:B:107:ARG:HA  | 5        | 0.15          |
| (1,1282) | 1:B:105:GLU:HA  | 1:B:106:GLU:H   | 9        | 0.15          |
| (1,1246) | 1:B:101:HIS:HB2 | 1:B:101:HIS:H   | 6        | 0.15          |
| (1,1234) | 1:B:101:HIS:HB3 | 1:B:92:LYS:HB2  | 3        | 0.15          |
| (1,1234) | 1:B:101:HIS:HB3 | 1:B:92:LYS:HB3  | 3        | 0.15          |
| (1,1229) | 1:B:100:VAL:H   | 1:B:100:VAL:HB  | 5        | 0.15          |
| (1,1227) | 1:B:100:VAL:HA  | 1:B:100:VAL:H   | 8        | 0.15          |
| (1,1208) | 1:B:98:ILE:HB   | 1:B:99:GLU:H    | 2        | 0.15          |
| (1,1208) | 1:B:98:ILE:HB   | 1:B:99:GLU:H    | 3        | 0.15          |
| (1,1206) | 1:B:98:ILE:HB   | 1:B:98:ILE:H    | 4        | 0.15          |
| (1,1206) | 1:B:98:ILE:HB   | 1:B:98:ILE:H    | 7        | 0.15          |
| (1,1206) | 1:B:98:ILE:HB   | 1:B:98:ILE:H    | 9        | 0.15          |
| (1,1202) | 1:B:98:ILE:H    | 1:B:97:VAL:H    | 9        | 0.15          |
| (1,1193) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA   | 3        | 0.15          |
| (1,1192) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA   | 3        | 0.15          |
| (1,1160) | 1:B:94:LEU:H    | 1:B:95:GLY:H    | 5        | 0.15          |
| (1,1142) | 1:B:92:LYS:H    | 1:B:92:LYS:HG2  | 2        | 0.15          |
| (1,1142) | 1:B:92:LYS:H    | 1:B:92:LYS:HG3  | 2        | 0.15          |
| (1,111)  | 1:A:77:VAL:HG11 | 1:A:122:TYR:HE1 | 8        | 0.15          |
| (1,111)  | 1:A:77:VAL:HG11 | 1:A:122:TYR:HE2 | 8        | 0.15          |
| (1,111)  | 1:A:77:VAL:HG12 | 1:A:122:TYR:HE1 | 8        | 0.15          |
| (1,111)  | 1:A:77:VAL:HG12 | 1:A:122:TYR:HE2 | 8        | 0.15          |
| (1,111)  | 1:A:77:VAL:HG13 | 1:A:122:TYR:HE1 | 8        | 0.15          |
| (1,111)  | 1:A:77:VAL:HG13 | 1:A:122:TYR:HE2 | 8        | 0.15          |
| (1,1109) | 1:B:89:LEU:H    | 1:B:88:GLU:H    | 8        | 0.15          |
| (1,1108) | 1:B:89:LEU:H    | 1:B:88:GLU:H    | 8        | 0.15          |
| (1,1106) | 1:B:89:LEU:H    | 1:B:87:GLU:HA   | 3        | 0.15          |
| (1,1103) | 1:B:89:LEU:HD21 | 1:B:85:SER:HB3  | 5        | 0.15          |
| (1,1103) | 1:B:89:LEU:HD22 | 1:B:85:SER:HB3  | 5        | 0.15          |
| (1,1103) | 1:B:89:LEU:HD23 | 1:B:85:SER:HB3  | 5        | 0.15          |
| (1,1102) | 1:B:88:GLU:H    | 1:B:89:LEU:HB2  | 5        | 0.15          |
| (1,1102) | 1:B:88:GLU:H    | 1:B:89:LEU:HB3  | 5        | 0.15          |
| (1,1098) | 1:B:87:GLU:HB2  | 1:B:89:LEU:H    | 1        | 0.15          |
| (1,1098) | 1:B:87:GLU:HB3  | 1:B:89:LEU:H    | 1        | 0.15          |
| (1,1045) | 1:B:83:HIS:HB3  | 1:B:83:HIS:H    | 8        | 0.15          |
| (1,103)  | 1:A:77:VAL:H    | 1:A:78:ASN:H    | 1        | 0.15          |
| (1,103)  | 1:A:77:VAL:H    | 1:A:78:ASN:H    | 3        | 0.15          |
| (1,990)  | 1:B:78:ASN:HB3  | 1:B:78:ASN:H    | 3        | 0.14          |
| (1,924)  | 1:B:75:PHE:H    | 1:B:149:ARG:H   | 9        | 0.14          |
| (1,896)  | 1:B:72:LYS:HB2  | 1:B:72:LYS:H    | 4        | 0.14          |
| (1,896)  | 1:B:72:LYS:HB3  | 1:B:72:LYS:H    | 4        | 0.14          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,895) | 1:B:72:LYS:H     | 1:B:72:LYS:HA   | 5        | 0.14          |
| (1,860) | 1:A:150:LYS:H    | 1:A:151:GLN:H   | 7        | 0.14          |
| (1,854) | 1:A:148:PRO:HB2  | 1:A:149:ARG:H   | 9        | 0.14          |
| (1,854) | 1:A:148:PRO:HB3  | 1:A:149:ARG:H   | 9        | 0.14          |
| (1,853) | 1:A:148:PRO:HA   | 1:A:148:PRO:HG2 | 6        | 0.14          |
| (1,853) | 1:A:148:PRO:HA   | 1:A:148:PRO:HG3 | 6        | 0.14          |
| (1,853) | 1:A:148:PRO:HA   | 1:A:148:PRO:HG2 | 8        | 0.14          |
| (1,853) | 1:A:148:PRO:HA   | 1:A:148:PRO:HG3 | 8        | 0.14          |
| (1,838) | 1:A:146:ASP:HB3  | 1:A:146:ASP:H   | 1        | 0.14          |
| (1,835) | 1:A:146:ASP:HB2  | 1:A:146:ASP:HA  | 9        | 0.14          |
| (1,834) | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 3        | 0.14          |
| (1,833) | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 3        | 0.14          |
| (1,832) | 1:A:146:ASP:HB2  | 1:A:146:ASP:HA  | 9        | 0.14          |
| (1,763) | 1:A:138:SER:H    | 1:A:142:VAL:H   | 3        | 0.14          |
| (1,760) | 1:A:138:SER:H    | 1:A:142:VAL:H   | 3        | 0.14          |
| (1,742) | 1:A:135:SER:HA   | 1:A:145:VAL:HA  | 1        | 0.14          |
| (1,740) | 1:A:135:SER:HA   | 1:A:145:VAL:HA  | 1        | 0.14          |
| (1,700) | 1:A:132:THR:HG21 | 1:A:132:THR:H   | 4        | 0.14          |
| (1,700) | 1:A:132:THR:HG22 | 1:A:132:THR:H   | 4        | 0.14          |
| (1,700) | 1:A:132:THR:HG23 | 1:A:132:THR:H   | 4        | 0.14          |
| (1,681) | 1:A:128:VAL:H    | 1:A:150:LYS:HD2 | 5        | 0.14          |
| (1,681) | 1:A:128:VAL:H    | 1:A:150:LYS:HD3 | 5        | 0.14          |
| (1,660) | 1:A:126:ALA:HA   | 1:A:128:VAL:H   | 6        | 0.14          |
| (1,614) | 1:A:124:ILE:HD11 | 1:A:96:ASP:H    | 5        | 0.14          |
| (1,614) | 1:A:124:ILE:HD12 | 1:A:96:ASP:H    | 5        | 0.14          |
| (1,614) | 1:A:124:ILE:HD13 | 1:A:96:ASP:H    | 5        | 0.14          |
| (1,606) | 1:A:123:ARG:HB2  | 1:A:123:ARG:HD2 | 6        | 0.14          |
| (1,606) | 1:A:123:ARG:HB2  | 1:A:123:ARG:HD3 | 6        | 0.14          |
| (1,596) | 1:A:122:TYR:HA   | 1:A:122:TYR:H   | 5        | 0.14          |
| (1,57)  | 1:A:75:PHE:H     | 1:A:149:ARG:H   | 9        | 0.14          |
| (1,553) | 1:A:118:PHE:HD1  | 1:A:103:LYS:H   | 1        | 0.14          |
| (1,553) | 1:A:118:PHE:HD2  | 1:A:103:LYS:H   | 1        | 0.14          |
| (1,535) | 1:A:116:ARG:H    | 1:A:104:HIS:H   | 8        | 0.14          |
| (1,534) | 1:A:116:ARG:H    | 1:A:104:HIS:H   | 8        | 0.14          |
| (1,521) | 1:A:115:SER:HB2  | 1:A:105:GLU:HB2 | 5        | 0.14          |
| (1,521) | 1:A:115:SER:HB2  | 1:A:105:GLU:HB3 | 5        | 0.14          |
| (1,459) | 1:A:111:HIS:H    | 1:A:110:GLU:H   | 8        | 0.14          |
| (1,458) | 1:A:111:HIS:H    | 1:A:110:GLU:H   | 8        | 0.14          |
| (1,454) | 1:A:110:GLU:H    | 1:A:110:GLU:HA  | 2        | 0.14          |
| (1,442) | 1:A:108:GLN:HA   | 1:A:108:GLN:HB2 | 3        | 0.14          |
| (1,442) | 1:A:108:GLN:HA   | 1:A:108:GLN:HB3 | 3        | 0.14          |
| (1,442) | 1:A:108:GLN:HA   | 1:A:108:GLN:HB2 | 7        | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,442)  | 1:A:108:GLN:HA   | 1:A:108:GLN:HB3 | 7        | 0.14          |
| (1,442)  | 1:A:108:GLN:HA   | 1:A:108:GLN:HB2 | 9        | 0.14          |
| (1,442)  | 1:A:108:GLN:HA   | 1:A:108:GLN:HB3 | 9        | 0.14          |
| (1,427)  | 1:A:107:ARG:HB3  | 1:A:107:ARG:H   | 8        | 0.14          |
| (1,424)  | 1:A:107:ARG:HG2  | 1:A:107:ARG:HA  | 2        | 0.14          |
| (1,424)  | 1:A:107:ARG:HG3  | 1:A:107:ARG:HA  | 2        | 0.14          |
| (1,411)  | 1:A:105:GLU:HB2  | 1:A:105:GLU:H   | 6        | 0.14          |
| (1,411)  | 1:A:105:GLU:HB3  | 1:A:105:GLU:H   | 6        | 0.14          |
| (1,411)  | 1:A:105:GLU:HB2  | 1:A:105:GLU:H   | 9        | 0.14          |
| (1,411)  | 1:A:105:GLU:HB3  | 1:A:105:GLU:H   | 9        | 0.14          |
| (1,400)  | 1:A:104:HIS:HA   | 1:A:84:PHE:HE1  | 1        | 0.14          |
| (1,400)  | 1:A:104:HIS:HA   | 1:A:84:PHE:HE2  | 1        | 0.14          |
| (1,367)  | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB2  | 5        | 0.14          |
| (1,367)  | 1:A:101:HIS:HB3  | 1:A:92:LYS:HB3  | 5        | 0.14          |
| (1,341)  | 1:A:98:ILE:HB    | 1:A:99:GLU:H    | 1        | 0.14          |
| (1,341)  | 1:A:98:ILE:HB    | 1:A:99:GLU:H    | 3        | 0.14          |
| (1,335)  | 1:A:98:ILE:H     | 1:A:97:VAL:H    | 5        | 0.14          |
| (1,326)  | 1:A:97:VAL:HB    | 1:A:97:VAL:HA   | 4        | 0.14          |
| (1,325)  | 1:A:97:VAL:HB    | 1:A:97:VAL:HA   | 4        | 0.14          |
| (1,29)   | 1:A:72:LYS:HB2   | 1:A:72:LYS:H    | 4        | 0.14          |
| (1,29)   | 1:A:72:LYS:HB3   | 1:A:72:LYS:H    | 4        | 0.14          |
| (1,28)   | 1:A:72:LYS:H     | 1:A:72:LYS:HA   | 5        | 0.14          |
| (1,257)  | 1:A:89:LEU:HD11  | 1:A:102:GLY:HA2 | 4        | 0.14          |
| (1,257)  | 1:A:89:LEU:HD12  | 1:A:102:GLY:HA2 | 4        | 0.14          |
| (1,257)  | 1:A:89:LEU:HD13  | 1:A:102:GLY:HA2 | 4        | 0.14          |
| (1,250)  | 1:A:89:LEU:HD21  | 1:A:89:LEU:H    | 1        | 0.14          |
| (1,250)  | 1:A:89:LEU:HD22  | 1:A:89:LEU:H    | 1        | 0.14          |
| (1,250)  | 1:A:89:LEU:HD23  | 1:A:89:LEU:H    | 1        | 0.14          |
| (1,1721) | 1:B:148:PRO:HB2  | 1:B:149:ARG:H   | 9        | 0.14          |
| (1,1721) | 1:B:148:PRO:HB3  | 1:B:149:ARG:H   | 9        | 0.14          |
| (1,1720) | 1:B:148:PRO:HA   | 1:B:148:PRO:HG2 | 8        | 0.14          |
| (1,1720) | 1:B:148:PRO:HA   | 1:B:148:PRO:HG3 | 8        | 0.14          |
| (1,1705) | 1:B:146:ASP:HB3  | 1:B:146:ASP:H   | 1        | 0.14          |
| (1,1702) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 9        | 0.14          |
| (1,1701) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA  | 3        | 0.14          |
| (1,1700) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA  | 3        | 0.14          |
| (1,1699) | 1:B:146:ASP:HB2  | 1:B:146:ASP:HA  | 9        | 0.14          |
| (1,1676) | 1:B:144:THR:HG21 | 1:B:146:ASP:HB3 | 4        | 0.14          |
| (1,1676) | 1:B:144:THR:HG22 | 1:B:146:ASP:HB3 | 4        | 0.14          |
| (1,1676) | 1:B:144:THR:HG23 | 1:B:146:ASP:HB3 | 4        | 0.14          |
| (1,1645) | 1:B:142:VAL:H    | 1:B:141:GLY:H   | 5        | 0.14          |
| (1,1644) | 1:B:142:VAL:H    | 1:B:141:GLY:H   | 5        | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1630) | 1:B:138:SER:H    | 1:B:142:VAL:H   | 3        | 0.14          |
| (1,1627) | 1:B:138:SER:H    | 1:B:142:VAL:H   | 3        | 0.14          |
| (1,1609) | 1:B:135:SER:HA   | 1:B:145:VAL:HA  | 1        | 0.14          |
| (1,1607) | 1:B:135:SER:HA   | 1:B:145:VAL:HA  | 1        | 0.14          |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD2 | 5        | 0.14          |
| (1,1548) | 1:B:128:VAL:H    | 1:B:150:LYS:HD3 | 5        | 0.14          |
| (1,1527) | 1:B:126:ALA:HA   | 1:B:128:VAL:H   | 6        | 0.14          |
| (1,1481) | 1:B:124:ILE:HD11 | 1:B:96:ASP:H    | 5        | 0.14          |
| (1,1481) | 1:B:124:ILE:HD12 | 1:B:96:ASP:H    | 5        | 0.14          |
| (1,1481) | 1:B:124:ILE:HD13 | 1:B:96:ASP:H    | 5        | 0.14          |
| (1,1473) | 1:B:123:ARG:HB2  | 1:B:123:ARG:HD2 | 6        | 0.14          |
| (1,1473) | 1:B:123:ARG:HB2  | 1:B:123:ARG:HD3 | 6        | 0.14          |
| (1,1463) | 1:B:122:TYR:HA   | 1:B:122:TYR:H   | 5        | 0.14          |
| (1,1402) | 1:B:116:ARG:H    | 1:B:104:HIS:H   | 8        | 0.14          |
| (1,1401) | 1:B:116:ARG:H    | 1:B:104:HIS:H   | 8        | 0.14          |
| (1,1388) | 1:B:115:SER:HB2  | 1:B:105:GLU:HB2 | 5        | 0.14          |
| (1,1388) | 1:B:115:SER:HB2  | 1:B:105:GLU:HB3 | 5        | 0.14          |
| (1,1326) | 1:B:111:HIS:H    | 1:B:110:GLU:H   | 8        | 0.14          |
| (1,1325) | 1:B:111:HIS:H    | 1:B:110:GLU:H   | 8        | 0.14          |
| (1,1321) | 1:B:110:GLU:H    | 1:B:110:GLU:HA  | 2        | 0.14          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB2 | 3        | 0.14          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB3 | 3        | 0.14          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB2 | 7        | 0.14          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB3 | 7        | 0.14          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB2 | 9        | 0.14          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB3 | 9        | 0.14          |
| (1,1294) | 1:B:107:ARG:HB3  | 1:B:107:ARG:H   | 8        | 0.14          |
| (1,1291) | 1:B:107:ARG:HG2  | 1:B:107:ARG:HA  | 2        | 0.14          |
| (1,1291) | 1:B:107:ARG:HG3  | 1:B:107:ARG:HA  | 2        | 0.14          |
| (1,1278) | 1:B:105:GLU:HB2  | 1:B:105:GLU:H   | 6        | 0.14          |
| (1,1278) | 1:B:105:GLU:HB3  | 1:B:105:GLU:H   | 6        | 0.14          |
| (1,1278) | 1:B:105:GLU:HB2  | 1:B:105:GLU:H   | 9        | 0.14          |
| (1,1278) | 1:B:105:GLU:HB3  | 1:B:105:GLU:H   | 9        | 0.14          |
| (1,1267) | 1:B:104:HIS:HA   | 1:B:84:PHE:HE1  | 1        | 0.14          |
| (1,1267) | 1:B:104:HIS:HA   | 1:B:84:PHE:HE2  | 1        | 0.14          |
| (1,1262) | 1:B:103:LYS:HG2  | 1:B:103:LYS:H   | 8        | 0.14          |
| (1,1262) | 1:B:103:LYS:HG3  | 1:B:103:LYS:H   | 8        | 0.14          |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB2  | 5        | 0.14          |
| (1,1234) | 1:B:101:HIS:HB3  | 1:B:92:LYS:HB3  | 5        | 0.14          |
| (1,123)  | 1:A:78:ASN:HB3   | 1:A:78:ASN:H    | 3        | 0.14          |
| (1,1208) | 1:B:98:ILE:HB    | 1:B:99:GLU:H    | 1        | 0.14          |
| (1,1202) | 1:B:98:ILE:H     | 1:B:97:VAL:H    | 5        | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1193) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA    | 4        | 0.14          |
| (1,1193) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA    | 5        | 0.14          |
| (1,1192) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA    | 4        | 0.14          |
| (1,1192) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA    | 5        | 0.14          |
| (1,1124) | 1:B:89:LEU:HD11 | 1:B:102:GLY:HA2  | 4        | 0.14          |
| (1,1124) | 1:B:89:LEU:HD12 | 1:B:102:GLY:HA2  | 4        | 0.14          |
| (1,1124) | 1:B:89:LEU:HD13 | 1:B:102:GLY:HA2  | 4        | 0.14          |
| (1,1117) | 1:B:89:LEU:HD21 | 1:B:89:LEU:H     | 1        | 0.14          |
| (1,1117) | 1:B:89:LEU:HD22 | 1:B:89:LEU:H     | 1        | 0.14          |
| (1,1117) | 1:B:89:LEU:HD23 | 1:B:89:LEU:H     | 1        | 0.14          |
| (1,1053) | 1:B:83:HIS:HB2  | 1:B:104:HIS:HB2  | 4        | 0.14          |
| (1,102)  | 1:A:77:VAL:HG11 | 1:A:78:ASN:H     | 3        | 0.14          |
| (1,102)  | 1:A:77:VAL:HG12 | 1:A:78:ASN:H     | 3        | 0.14          |
| (1,102)  | 1:A:77:VAL:HG13 | 1:A:78:ASN:H     | 3        | 0.14          |
| (1,983)  | 1:B:77:VAL:H    | 1:B:145:VAL:H    | 9        | 0.13          |
| (1,944)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB3  | 1        | 0.13          |
| (1,940)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2  | 1        | 0.13          |
| (1,937)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2  | 1        | 0.13          |
| (1,934)  | 1:B:76:SER:HB2  | 1:B:146:ASP:HB2  | 1        | 0.13          |
| (1,923)  | 1:B:75:PHE:HD1  | 1:B:148:PRO:HA   | 3        | 0.13          |
| (1,923)  | 1:B:75:PHE:HD2  | 1:B:148:PRO:HA   | 3        | 0.13          |
| (1,918)  | 1:B:75:PHE:HA   | 1:B:76:SER:H     | 4        | 0.13          |
| (1,918)  | 1:B:75:PHE:HA   | 1:B:76:SER:H     | 9        | 0.13          |
| (1,915)  | 1:B:75:PHE:HA   | 1:B:75:PHE:HB3   | 8        | 0.13          |
| (1,888)  | 1:B:70:LEU:HD11 | 1:B:71:GLU:H     | 2        | 0.13          |
| (1,888)  | 1:B:70:LEU:HD12 | 1:B:71:GLU:H     | 2        | 0.13          |
| (1,888)  | 1:B:70:LEU:HD13 | 1:B:71:GLU:H     | 2        | 0.13          |
| (1,888)  | 1:B:70:LEU:HD21 | 1:B:71:GLU:H     | 2        | 0.13          |
| (1,888)  | 1:B:70:LEU:HD22 | 1:B:71:GLU:H     | 2        | 0.13          |
| (1,888)  | 1:B:70:LEU:HD23 | 1:B:71:GLU:H     | 2        | 0.13          |
| (1,874)  | 1:B:68:MET:HA   | 1:B:68:MET:HG2   | 2        | 0.13          |
| (1,874)  | 1:B:68:MET:HA   | 1:B:68:MET:HG3   | 2        | 0.13          |
| (1,874)  | 1:B:68:MET:HA   | 1:B:68:MET:HG2   | 7        | 0.13          |
| (1,874)  | 1:B:68:MET:HA   | 1:B:68:MET:HG3   | 7        | 0.13          |
| (1,867)  | 1:A:152:VAL:H   | 1:A:152:VAL:HG11 | 8        | 0.13          |
| (1,867)  | 1:A:152:VAL:H   | 1:A:152:VAL:HG12 | 8        | 0.13          |
| (1,867)  | 1:A:152:VAL:H   | 1:A:152:VAL:HG13 | 8        | 0.13          |
| (1,867)  | 1:A:152:VAL:H   | 1:A:152:VAL:HG21 | 8        | 0.13          |
| (1,867)  | 1:A:152:VAL:H   | 1:A:152:VAL:HG22 | 8        | 0.13          |
| (1,867)  | 1:A:152:VAL:H   | 1:A:152:VAL:HG23 | 8        | 0.13          |
| (1,856)  | 1:A:150:LYS:H   | 1:A:149:ARG:H    | 1        | 0.13          |
| (1,847)  | 1:A:147:GLY:HA2 | 1:A:147:GLY:H    | 5        | 0.13          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,834) | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 5        | 0.13          |
| (1,834) | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 8        | 0.13          |
| (1,833) | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 5        | 0.13          |
| (1,833) | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 8        | 0.13          |
| (1,812) | 1:A:145:VAL:HB   | 1:A:135:SER:HA  | 8        | 0.13          |
| (1,802) | 1:A:144:THR:HB   | 1:A:144:THR:H   | 1        | 0.13          |
| (1,731) | 1:A:134:THR:HG21 | 1:A:135:SER:H   | 8        | 0.13          |
| (1,731) | 1:A:134:THR:HG22 | 1:A:135:SER:H   | 8        | 0.13          |
| (1,731) | 1:A:134:THR:HG23 | 1:A:135:SER:H   | 8        | 0.13          |
| (1,73)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2 | 1        | 0.13          |
| (1,70)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2 | 1        | 0.13          |
| (1,7)   | 1:A:68:MET:HA    | 1:A:68:MET:HG2  | 2        | 0.13          |
| (1,7)   | 1:A:68:MET:HA    | 1:A:68:MET:HG3  | 2        | 0.13          |
| (1,7)   | 1:A:68:MET:HA    | 1:A:68:MET:HG2  | 7        | 0.13          |
| (1,7)   | 1:A:68:MET:HA    | 1:A:68:MET:HG3  | 7        | 0.13          |
| (1,680) | 1:A:128:VAL:H    | 1:A:129:ASP:H   | 1        | 0.13          |
| (1,673) | 1:A:127:ASP:HB3  | 1:A:128:VAL:H   | 4        | 0.13          |
| (1,670) | 1:A:127:ASP:HB3  | 1:A:127:ASP:H   | 4        | 0.13          |
| (1,67)  | 1:A:76:SER:HB2   | 1:A:146:ASP:HB2 | 1        | 0.13          |
| (1,644) | 1:A:125:PRO:HD2  | 1:A:124:ILE:HB  | 2        | 0.13          |
| (1,615) | 1:A:124:ILE:HB   | 1:A:97:VAL:HA   | 4        | 0.13          |
| (1,606) | 1:A:123:ARG:HB2  | 1:A:123:ARG:HD2 | 1        | 0.13          |
| (1,606) | 1:A:123:ARG:HB2  | 1:A:123:ARG:HD3 | 1        | 0.13          |
| (1,606) | 1:A:123:ARG:HB2  | 1:A:123:ARG:HD2 | 7        | 0.13          |
| (1,606) | 1:A:123:ARG:HB2  | 1:A:123:ARG:HD3 | 7        | 0.13          |
| (1,56)  | 1:A:75:PHE:HD1   | 1:A:148:PRO:HA  | 3        | 0.13          |
| (1,56)  | 1:A:75:PHE:HD2   | 1:A:148:PRO:HA  | 3        | 0.13          |
| (1,541) | 1:A:117:GLU:HA   | 1:A:103:LYS:HG2 | 1        | 0.13          |
| (1,541) | 1:A:117:GLU:HA   | 1:A:103:LYS:HG3 | 1        | 0.13          |
| (1,541) | 1:A:117:GLU:HA   | 1:A:103:LYS:HG2 | 2        | 0.13          |
| (1,541) | 1:A:117:GLU:HA   | 1:A:103:LYS:HG3 | 2        | 0.13          |
| (1,535) | 1:A:116:ARG:H    | 1:A:104:HIS:H   | 7        | 0.13          |
| (1,534) | 1:A:116:ARG:H    | 1:A:104:HIS:H   | 7        | 0.13          |
| (1,532) | 1:A:115:SER:HB3  | 1:A:116:ARG:H   | 9        | 0.13          |
| (1,510) | 1:A:114:ILE:HG21 | 1:A:111:HIS:H   | 3        | 0.13          |
| (1,510) | 1:A:114:ILE:HG22 | 1:A:111:HIS:H   | 3        | 0.13          |
| (1,510) | 1:A:114:ILE:HG23 | 1:A:111:HIS:H   | 3        | 0.13          |
| (1,51)  | 1:A:75:PHE:HA    | 1:A:76:SER:H    | 4        | 0.13          |
| (1,51)  | 1:A:75:PHE:HA    | 1:A:76:SER:H    | 9        | 0.13          |
| (1,505) | 1:A:114:ILE:HD11 | 1:A:107:ARG:HG2 | 7        | 0.13          |
| (1,505) | 1:A:114:ILE:HD11 | 1:A:107:ARG:HG3 | 7        | 0.13          |
| (1,505) | 1:A:114:ILE:HD12 | 1:A:107:ARG:HG2 | 7        | 0.13          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,505) | 1:A:114:ILE:HD12 | 1:A:107:ARG:HG3 | 7        | 0.13          |
| (1,505) | 1:A:114:ILE:HD13 | 1:A:107:ARG:HG2 | 7        | 0.13          |
| (1,505) | 1:A:114:ILE:HD13 | 1:A:107:ARG:HG3 | 7        | 0.13          |
| (1,502) | 1:A:114:ILE:HD11 | 1:A:104:HIS:HB2 | 3        | 0.13          |
| (1,502) | 1:A:114:ILE:HD12 | 1:A:104:HIS:HB2 | 3        | 0.13          |
| (1,502) | 1:A:114:ILE:HD13 | 1:A:104:HIS:HB2 | 3        | 0.13          |
| (1,482) | 1:A:113:PHE:HD1  | 1:A:107:ARG:HA  | 6        | 0.13          |
| (1,482) | 1:A:113:PHE:HD2  | 1:A:107:ARG:HA  | 6        | 0.13          |
| (1,48)  | 1:A:75:PHE:HA    | 1:A:75:PHE:HB3  | 8        | 0.13          |
| (1,451) | 1:A:109:ASP:H    | 1:A:112:GLY:H   | 4        | 0.13          |
| (1,442) | 1:A:108:GLN:HA   | 1:A:108:GLN:HB2 | 6        | 0.13          |
| (1,442) | 1:A:108:GLN:HA   | 1:A:108:GLN:HB3 | 6        | 0.13          |
| (1,427) | 1:A:107:ARG:HB3  | 1:A:107:ARG:H   | 3        | 0.13          |
| (1,425) | 1:A:107:ARG:HA   | 1:A:107:ARG:H   | 6        | 0.13          |
| (1,424) | 1:A:107:ARG:HG2  | 1:A:107:ARG:HA  | 4        | 0.13          |
| (1,424) | 1:A:107:ARG:HG3  | 1:A:107:ARG:HA  | 4        | 0.13          |
| (1,417) | 1:A:105:GLU:HG2  | 1:A:106:GLU:H   | 9        | 0.13          |
| (1,417) | 1:A:105:GLU:HG3  | 1:A:106:GLU:H   | 9        | 0.13          |
| (1,415) | 1:A:105:GLU:HA   | 1:A:106:GLU:H   | 5        | 0.13          |
| (1,375) | 1:A:101:HIS:HB2  | 1:A:101:HIS:HA  | 1        | 0.13          |
| (1,375) | 1:A:101:HIS:HB2  | 1:A:101:HIS:HA  | 3        | 0.13          |
| (1,375) | 1:A:101:HIS:HB2  | 1:A:101:HIS:HA  | 6        | 0.13          |
| (1,374) | 1:A:101:HIS:HB2  | 1:A:101:HIS:HA  | 1        | 0.13          |
| (1,374) | 1:A:101:HIS:HB2  | 1:A:101:HIS:HA  | 3        | 0.13          |
| (1,374) | 1:A:101:HIS:HB2  | 1:A:101:HIS:HA  | 6        | 0.13          |
| (1,369) | 1:A:101:HIS:H    | 1:A:100:VAL:HA  | 7        | 0.13          |
| (1,346) | 1:A:98:ILE:H     | 1:A:122:TYR:H   | 1        | 0.13          |
| (1,345) | 1:A:98:ILE:H     | 1:A:122:TYR:H   | 1        | 0.13          |
| (1,341) | 1:A:98:ILE:HB    | 1:A:99:GLU:H    | 5        | 0.13          |
| (1,341) | 1:A:98:ILE:HB    | 1:A:99:GLU:H    | 8        | 0.13          |
| (1,326) | 1:A:97:VAL:HB    | 1:A:97:VAL:HA   | 2        | 0.13          |
| (1,326) | 1:A:97:VAL:HB    | 1:A:97:VAL:HA   | 9        | 0.13          |
| (1,325) | 1:A:97:VAL:HB    | 1:A:97:VAL:HA   | 2        | 0.13          |
| (1,325) | 1:A:97:VAL:HB    | 1:A:97:VAL:HA   | 9        | 0.13          |
| (1,259) | 1:A:89:LEU:HD11  | 1:A:103:LYS:H   | 6        | 0.13          |
| (1,259) | 1:A:89:LEU:HD12  | 1:A:103:LYS:H   | 6        | 0.13          |
| (1,259) | 1:A:89:LEU:HD13  | 1:A:103:LYS:H   | 6        | 0.13          |
| (1,259) | 1:A:89:LEU:HD11  | 1:A:103:LYS:H   | 8        | 0.13          |
| (1,259) | 1:A:89:LEU:HD12  | 1:A:103:LYS:H   | 8        | 0.13          |
| (1,259) | 1:A:89:LEU:HD13  | 1:A:103:LYS:H   | 8        | 0.13          |
| (1,252) | 1:A:89:LEU:H     | 1:A:90:LYS:H    | 3        | 0.13          |
| (1,245) | 1:A:89:LEU:HA    | 1:A:89:LEU:HD21 | 2        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD22  | 2        | 0.13          |
| (1,245)  | 1:A:89:LEU:HA    | 1:A:89:LEU:HD23  | 2        | 0.13          |
| (1,21)   | 1:A:70:LEU:HD11  | 1:A:71:GLU:H     | 2        | 0.13          |
| (1,21)   | 1:A:70:LEU:HD12  | 1:A:71:GLU:H     | 2        | 0.13          |
| (1,21)   | 1:A:70:LEU:HD13  | 1:A:71:GLU:H     | 2        | 0.13          |
| (1,21)   | 1:A:70:LEU:HD21  | 1:A:71:GLU:H     | 2        | 0.13          |
| (1,21)   | 1:A:70:LEU:HD22  | 1:A:71:GLU:H     | 2        | 0.13          |
| (1,21)   | 1:A:70:LEU:HD23  | 1:A:71:GLU:H     | 2        | 0.13          |
| (1,1734) | 1:B:152:VAL:H    | 1:B:152:VAL:HG11 | 8        | 0.13          |
| (1,1734) | 1:B:152:VAL:H    | 1:B:152:VAL:HG12 | 8        | 0.13          |
| (1,1734) | 1:B:152:VAL:H    | 1:B:152:VAL:HG13 | 8        | 0.13          |
| (1,1734) | 1:B:152:VAL:H    | 1:B:152:VAL:HG21 | 8        | 0.13          |
| (1,1734) | 1:B:152:VAL:H    | 1:B:152:VAL:HG22 | 8        | 0.13          |
| (1,1734) | 1:B:152:VAL:H    | 1:B:152:VAL:HG23 | 8        | 0.13          |
| (1,1727) | 1:B:150:LYS:H    | 1:B:151:GLN:H    | 7        | 0.13          |
| (1,1723) | 1:B:150:LYS:H    | 1:B:149:ARG:H    | 1        | 0.13          |
| (1,1720) | 1:B:148:PRO:HA   | 1:B:148:PRO:HG2  | 6        | 0.13          |
| (1,1720) | 1:B:148:PRO:HA   | 1:B:148:PRO:HG3  | 6        | 0.13          |
| (1,1714) | 1:B:147:GLY:HA2  | 1:B:147:GLY:H    | 5        | 0.13          |
| (1,1701) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA   | 5        | 0.13          |
| (1,1701) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA   | 8        | 0.13          |
| (1,1700) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA   | 5        | 0.13          |
| (1,1700) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA   | 8        | 0.13          |
| (1,1679) | 1:B:145:VAL:HB   | 1:B:135:SER:HA   | 8        | 0.13          |
| (1,1669) | 1:B:144:THR:HB   | 1:B:144:THR:H    | 1        | 0.13          |
| (1,160)  | 1:A:81:VAL:H     | 1:A:82:LYS:H     | 4        | 0.13          |
| (1,1598) | 1:B:134:THR:HG21 | 1:B:135:SER:H    | 8        | 0.13          |
| (1,1598) | 1:B:134:THR:HG22 | 1:B:135:SER:H    | 8        | 0.13          |
| (1,1598) | 1:B:134:THR:HG23 | 1:B:135:SER:H    | 8        | 0.13          |
| (1,1547) | 1:B:128:VAL:H    | 1:B:129:ASP:H    | 1        | 0.13          |
| (1,1540) | 1:B:127:ASP:HB3  | 1:B:128:VAL:H    | 4        | 0.13          |
| (1,1537) | 1:B:127:ASP:HB3  | 1:B:127:ASP:H    | 4        | 0.13          |
| (1,1511) | 1:B:125:PRO:HD2  | 1:B:124:ILE:HB   | 2        | 0.13          |
| (1,1482) | 1:B:124:ILE:HB   | 1:B:97:VAL:HA    | 4        | 0.13          |
| (1,1473) | 1:B:123:ARG:HB2  | 1:B:123:ARG:HD2  | 1        | 0.13          |
| (1,1473) | 1:B:123:ARG:HB2  | 1:B:123:ARG:HD3  | 1        | 0.13          |
| (1,1473) | 1:B:123:ARG:HB2  | 1:B:123:ARG:HD2  | 7        | 0.13          |
| (1,1473) | 1:B:123:ARG:HB2  | 1:B:123:ARG:HD3  | 7        | 0.13          |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG11  | 8        | 0.13          |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG12  | 8        | 0.13          |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG13  | 8        | 0.13          |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG21  | 8        | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG22 | 8        | 0.13          |
| (1,1449) | 1:B:121:LYS:HA   | 1:B:97:VAL:HG23 | 8        | 0.13          |
| (1,1420) | 1:B:118:PHE:HD1  | 1:B:103:LYS:H   | 1        | 0.13          |
| (1,1420) | 1:B:118:PHE:HD2  | 1:B:103:LYS:H   | 1        | 0.13          |
| (1,1408) | 1:B:117:GLU:HA   | 1:B:103:LYS:HG2 | 1        | 0.13          |
| (1,1408) | 1:B:117:GLU:HA   | 1:B:103:LYS:HG3 | 1        | 0.13          |
| (1,1408) | 1:B:117:GLU:HA   | 1:B:103:LYS:HG2 | 2        | 0.13          |
| (1,1408) | 1:B:117:GLU:HA   | 1:B:103:LYS:HG3 | 2        | 0.13          |
| (1,1402) | 1:B:116:ARG:H    | 1:B:104:HIS:H   | 7        | 0.13          |
| (1,1401) | 1:B:116:ARG:H    | 1:B:104:HIS:H   | 7        | 0.13          |
| (1,1399) | 1:B:115:SER:HB3  | 1:B:116:ARG:H   | 9        | 0.13          |
| (1,1377) | 1:B:114:ILE:HG21 | 1:B:111:HIS:H   | 3        | 0.13          |
| (1,1377) | 1:B:114:ILE:HG22 | 1:B:111:HIS:H   | 3        | 0.13          |
| (1,1377) | 1:B:114:ILE:HG23 | 1:B:111:HIS:H   | 3        | 0.13          |
| (1,1372) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HG2 | 7        | 0.13          |
| (1,1372) | 1:B:114:ILE:HD11 | 1:B:107:ARG:HG3 | 7        | 0.13          |
| (1,1372) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HG2 | 7        | 0.13          |
| (1,1372) | 1:B:114:ILE:HD12 | 1:B:107:ARG:HG3 | 7        | 0.13          |
| (1,1372) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HG2 | 7        | 0.13          |
| (1,1372) | 1:B:114:ILE:HD13 | 1:B:107:ARG:HG3 | 7        | 0.13          |
| (1,1369) | 1:B:114:ILE:HD11 | 1:B:104:HIS:HB2 | 3        | 0.13          |
| (1,1369) | 1:B:114:ILE:HD12 | 1:B:104:HIS:HB2 | 3        | 0.13          |
| (1,1369) | 1:B:114:ILE:HD13 | 1:B:104:HIS:HB2 | 3        | 0.13          |
| (1,1349) | 1:B:113:PHE:HD1  | 1:B:107:ARG:HA  | 6        | 0.13          |
| (1,1349) | 1:B:113:PHE:HD2  | 1:B:107:ARG:HA  | 6        | 0.13          |
| (1,1318) | 1:B:109:ASP:H    | 1:B:112:GLY:H   | 4        | 0.13          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB2 | 6        | 0.13          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB3 | 6        | 0.13          |
| (1,1294) | 1:B:107:ARG:HB3  | 1:B:107:ARG:H   | 3        | 0.13          |
| (1,1292) | 1:B:107:ARG:HA   | 1:B:107:ARG:H   | 6        | 0.13          |
| (1,1291) | 1:B:107:ARG:HG2  | 1:B:107:ARG:HA  | 4        | 0.13          |
| (1,1291) | 1:B:107:ARG:HG3  | 1:B:107:ARG:HA  | 4        | 0.13          |
| (1,1284) | 1:B:105:GLU:HG2  | 1:B:106:GLU:H   | 9        | 0.13          |
| (1,1284) | 1:B:105:GLU:HG3  | 1:B:106:GLU:H   | 9        | 0.13          |
| (1,1282) | 1:B:105:GLU:HA   | 1:B:106:GLU:H   | 5        | 0.13          |
| (1,1242) | 1:B:101:HIS:HB2  | 1:B:101:HIS:HA  | 1        | 0.13          |
| (1,1242) | 1:B:101:HIS:HB2  | 1:B:101:HIS:HA  | 3        | 0.13          |
| (1,1242) | 1:B:101:HIS:HB2  | 1:B:101:HIS:HA  | 6        | 0.13          |
| (1,1241) | 1:B:101:HIS:HB2  | 1:B:101:HIS:HA  | 1        | 0.13          |
| (1,1241) | 1:B:101:HIS:HB2  | 1:B:101:HIS:HA  | 3        | 0.13          |
| (1,1241) | 1:B:101:HIS:HB2  | 1:B:101:HIS:HA  | 6        | 0.13          |
| (1,1236) | 1:B:101:HIS:H    | 1:B:100:VAL:HA  | 7        | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1225) | 1:B:100:VAL:HG11 | 1:B:92:LYS:H    | 9        | 0.13          |
| (1,1225) | 1:B:100:VAL:HG12 | 1:B:92:LYS:H    | 9        | 0.13          |
| (1,1225) | 1:B:100:VAL:HG13 | 1:B:92:LYS:H    | 9        | 0.13          |
| (1,1213) | 1:B:98:ILE:H     | 1:B:122:TYR:H   | 1        | 0.13          |
| (1,1212) | 1:B:98:ILE:H     | 1:B:122:TYR:H   | 1        | 0.13          |
| (1,1208) | 1:B:98:ILE:HB    | 1:B:99:GLU:H    | 5        | 0.13          |
| (1,1208) | 1:B:98:ILE:HB    | 1:B:99:GLU:H    | 8        | 0.13          |
| (1,1193) | 1:B:97:VAL:HB    | 1:B:97:VAL:HA   | 2        | 0.13          |
| (1,1193) | 1:B:97:VAL:HB    | 1:B:97:VAL:HA   | 9        | 0.13          |
| (1,1192) | 1:B:97:VAL:HB    | 1:B:97:VAL:HA   | 2        | 0.13          |
| (1,1192) | 1:B:97:VAL:HB    | 1:B:97:VAL:HA   | 9        | 0.13          |
| (1,1116) | 1:A:77:VAL:H     | 1:A:145:VAL:H   | 9        | 0.13          |
| (1,1126) | 1:B:89:LEU:HD11  | 1:B:103:LYS:H   | 6        | 0.13          |
| (1,1126) | 1:B:89:LEU:HD12  | 1:B:103:LYS:H   | 6        | 0.13          |
| (1,1126) | 1:B:89:LEU:HD13  | 1:B:103:LYS:H   | 6        | 0.13          |
| (1,1126) | 1:B:89:LEU:HD11  | 1:B:103:LYS:H   | 8        | 0.13          |
| (1,1126) | 1:B:89:LEU:HD12  | 1:B:103:LYS:H   | 8        | 0.13          |
| (1,1126) | 1:B:89:LEU:HD13  | 1:B:103:LYS:H   | 8        | 0.13          |
| (1,1119) | 1:B:89:LEU:H     | 1:B:90:LYS:H    | 3        | 0.13          |
| (1,1112) | 1:B:89:LEU:HA    | 1:B:89:LEU:HD21 | 2        | 0.13          |
| (1,1112) | 1:B:89:LEU:HA    | 1:B:89:LEU:HD22 | 2        | 0.13          |
| (1,1112) | 1:B:89:LEU:HA    | 1:B:89:LEU:HD23 | 2        | 0.13          |
| (1,1027) | 1:B:81:VAL:H     | 1:B:82:LYS:H    | 4        | 0.13          |
| (1,997)  | 1:B:78:ASN:HB2   | 1:B:79:LEU:H    | 3        | 0.12          |
| (1,997)  | 1:B:78:ASN:HB2   | 1:B:79:LEU:H    | 5        | 0.12          |
| (1,996)  | 1:B:78:ASN:HB3   | 1:B:79:LEU:H    | 5        | 0.12          |
| (1,990)  | 1:B:78:ASN:HB3   | 1:B:78:ASN:H    | 4        | 0.12          |
| (1,990)  | 1:B:78:ASN:HB3   | 1:B:78:ASN:H    | 5        | 0.12          |
| (1,961)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HB   | 6        | 0.12          |
| (1,957)  | 1:B:77:VAL:HA    | 1:B:77:VAL:HB   | 6        | 0.12          |
| (1,945)  | 1:B:76:SER:HA    | 1:B:146:ASP:HA  | 4        | 0.12          |
| (1,942)  | 1:B:76:SER:HB3   | 1:B:146:ASP:HB3 | 9        | 0.12          |
| (1,941)  | 1:B:76:SER:HA    | 1:B:146:ASP:HA  | 4        | 0.12          |
| (1,94)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HB   | 6        | 0.12          |
| (1,90)   | 1:A:77:VAL:HA    | 1:A:77:VAL:HB   | 6        | 0.12          |
| (1,896)  | 1:B:72:LYS:HB2   | 1:B:72:LYS:H    | 3        | 0.12          |
| (1,896)  | 1:B:72:LYS:HB3   | 1:B:72:LYS:H    | 3        | 0.12          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD11 | 8        | 0.12          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD12 | 8        | 0.12          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD13 | 8        | 0.12          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD21 | 8        | 0.12          |
| (1,879)  | 1:B:68:MET:HE1   | 1:B:70:LEU:HD22 | 8        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,879) | 1:B:68:MET:HE1  | 1:B:70:LEU:HD23 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE2  | 1:B:70:LEU:HD11 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE2  | 1:B:70:LEU:HD12 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE2  | 1:B:70:LEU:HD13 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE2  | 1:B:70:LEU:HD21 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE2  | 1:B:70:LEU:HD22 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE2  | 1:B:70:LEU:HD23 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE3  | 1:B:70:LEU:HD11 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE3  | 1:B:70:LEU:HD12 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE3  | 1:B:70:LEU:HD13 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE3  | 1:B:70:LEU:HD21 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE3  | 1:B:70:LEU:HD22 | 8        | 0.12          |
| (1,879) | 1:B:68:MET:HE3  | 1:B:70:LEU:HD23 | 8        | 0.12          |
| (1,874) | 1:B:68:MET:HA   | 1:B:68:MET:HG2  | 9        | 0.12          |
| (1,874) | 1:B:68:MET:HA   | 1:B:68:MET:HG3  | 9        | 0.12          |
| (1,808) | 1:A:144:THR:H   | 1:A:145:VAL:H   | 1        | 0.12          |
| (1,808) | 1:A:144:THR:H   | 1:A:145:VAL:H   | 7        | 0.12          |
| (1,803) | 1:A:144:THR:H   | 1:A:145:VAL:H   | 1        | 0.12          |
| (1,803) | 1:A:144:THR:H   | 1:A:145:VAL:H   | 7        | 0.12          |
| (1,787) | 1:A:143:LEU:H   | 1:A:79:LEU:H    | 7        | 0.12          |
| (1,78)  | 1:A:76:SER:HA   | 1:A:146:ASP:HA  | 4        | 0.12          |
| (1,77)  | 1:A:76:SER:HB2  | 1:A:146:ASP:HB3 | 1        | 0.12          |
| (1,74)  | 1:A:76:SER:HA   | 1:A:146:ASP:HA  | 4        | 0.12          |
| (1,7)   | 1:A:68:MET:HA   | 1:A:68:MET:HG2  | 9        | 0.12          |
| (1,7)   | 1:A:68:MET:HA   | 1:A:68:MET:HG3  | 9        | 0.12          |
| (1,681) | 1:A:128:VAL:H   | 1:A:150:LYS:HD2 | 3        | 0.12          |
| (1,681) | 1:A:128:VAL:H   | 1:A:150:LYS:HD3 | 3        | 0.12          |
| (1,681) | 1:A:128:VAL:H   | 1:A:150:LYS:HD2 | 6        | 0.12          |
| (1,681) | 1:A:128:VAL:H   | 1:A:150:LYS:HD3 | 6        | 0.12          |
| (1,680) | 1:A:128:VAL:H   | 1:A:129:ASP:H   | 6        | 0.12          |
| (1,662) | 1:A:127:ASP:H   | 1:A:125:PRO:HB2 | 2        | 0.12          |
| (1,662) | 1:A:127:ASP:H   | 1:A:125:PRO:HB3 | 2        | 0.12          |
| (1,607) | 1:A:123:ARG:HB3 | 1:A:123:ARG:HD2 | 3        | 0.12          |
| (1,607) | 1:A:123:ARG:HB3 | 1:A:123:ARG:HD3 | 3        | 0.12          |
| (1,598) | 1:A:122:TYR:HB2 | 1:A:122:TYR:H   | 1        | 0.12          |
| (1,598) | 1:A:122:TYR:HB3 | 1:A:122:TYR:H   | 1        | 0.12          |
| (1,597) | 1:A:122:TYR:HB2 | 1:A:122:TYR:H   | 1        | 0.12          |
| (1,597) | 1:A:122:TYR:HB3 | 1:A:122:TYR:H   | 1        | 0.12          |
| (1,596) | 1:A:122:TYR:HA  | 1:A:122:TYR:H   | 4        | 0.12          |
| (1,589) | 1:A:122:TYR:HE1 | 1:A:98:ILE:HG21 | 8        | 0.12          |
| (1,589) | 1:A:122:TYR:HE1 | 1:A:98:ILE:HG22 | 8        | 0.12          |
| (1,589) | 1:A:122:TYR:HE1 | 1:A:98:ILE:HG23 | 8        | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,589)  | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG21 | 8        | 0.12          |
| (1,589)  | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG22 | 8        | 0.12          |
| (1,589)  | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG23 | 8        | 0.12          |
| (1,559)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HD1 | 2        | 0.12          |
| (1,559)  | 1:A:118:PHE:HA   | 1:A:118:PHE:HD2 | 2        | 0.12          |
| (1,532)  | 1:A:115:SER:HB3  | 1:A:116:ARG:H   | 2        | 0.12          |
| (1,465)  | 1:A:111:HIS:HB2  | 1:A:111:HIS:H   | 5        | 0.12          |
| (1,447)  | 1:A:109:ASP:H    | 1:A:109:ASP:HB2 | 3        | 0.12          |
| (1,447)  | 1:A:109:ASP:H    | 1:A:109:ASP:HB3 | 3        | 0.12          |
| (1,442)  | 1:A:108:GLN:HA   | 1:A:108:GLN:HB2 | 4        | 0.12          |
| (1,442)  | 1:A:108:GLN:HA   | 1:A:108:GLN:HB3 | 4        | 0.12          |
| (1,419)  | 1:A:105:GLU:HA   | 1:A:116:ARG:H   | 8        | 0.12          |
| (1,414)  | 1:A:105:GLU:HG2  | 1:A:105:GLU:H   | 8        | 0.12          |
| (1,414)  | 1:A:105:GLU:HG3  | 1:A:105:GLU:H   | 8        | 0.12          |
| (1,395)  | 1:A:103:LYS:HG2  | 1:A:103:LYS:H   | 7        | 0.12          |
| (1,395)  | 1:A:103:LYS:HG3  | 1:A:103:LYS:H   | 7        | 0.12          |
| (1,390)  | 1:A:102:GLY:HA2  | 1:A:103:LYS:H   | 6        | 0.12          |
| (1,372)  | 1:A:101:HIS:HA   | 1:A:101:HIS:HD2 | 1        | 0.12          |
| (1,372)  | 1:A:101:HIS:HA   | 1:A:101:HIS:HD2 | 2        | 0.12          |
| (1,358)  | 1:A:100:VAL:HG11 | 1:A:92:LYS:H    | 9        | 0.12          |
| (1,358)  | 1:A:100:VAL:HG12 | 1:A:92:LYS:H    | 9        | 0.12          |
| (1,358)  | 1:A:100:VAL:HG13 | 1:A:92:LYS:H    | 9        | 0.12          |
| (1,341)  | 1:A:98:ILE:HB    | 1:A:99:GLU:H    | 7        | 0.12          |
| (1,341)  | 1:A:98:ILE:HB    | 1:A:99:GLU:H    | 9        | 0.12          |
| (1,335)  | 1:A:98:ILE:H     | 1:A:97:VAL:H    | 1        | 0.12          |
| (1,335)  | 1:A:98:ILE:H     | 1:A:97:VAL:H    | 3        | 0.12          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD11 | 6        | 0.12          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD12 | 6        | 0.12          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD13 | 6        | 0.12          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD21 | 6        | 0.12          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD22 | 6        | 0.12          |
| (1,297)  | 1:A:95:GLY:HA2   | 1:A:94:LEU:HD23 | 6        | 0.12          |
| (1,29)   | 1:A:72:LYS:HB2   | 1:A:72:LYS:H    | 3        | 0.12          |
| (1,29)   | 1:A:72:LYS:HB3   | 1:A:72:LYS:H    | 3        | 0.12          |
| (1,280)  | 1:A:92:LYS:H     | 1:A:100:VAL:HA  | 4        | 0.12          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG21 | 2        | 0.12          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG22 | 2        | 0.12          |
| (1,268)  | 1:A:91:VAL:H     | 1:A:91:VAL:HG23 | 2        | 0.12          |
| (1,1744) | 1:A:114:ILE:HA   | 1:B:120:ARG:HB2 | 9        | 0.12          |
| (1,1744) | 1:A:114:ILE:HA   | 1:B:120:ARG:HB3 | 9        | 0.12          |
| (1,1675) | 1:B:144:THR:H    | 1:B:145:VAL:H   | 1        | 0.12          |
| (1,1675) | 1:B:144:THR:H    | 1:B:145:VAL:H   | 7        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1670) | 1:B:144:THR:H   | 1:B:145:VAL:H   | 1        | 0.12          |
| (1,1670) | 1:B:144:THR:H   | 1:B:145:VAL:H   | 7        | 0.12          |
| (1,1654) | 1:B:143:LEU:H   | 1:B:79:LEU:H    | 7        | 0.12          |
| (1,163)  | 1:A:81:VAL:HG21 | 1:A:83:HIS:H    | 6        | 0.12          |
| (1,163)  | 1:A:81:VAL:HG22 | 1:A:83:HIS:H    | 6        | 0.12          |
| (1,163)  | 1:A:81:VAL:HG23 | 1:A:83:HIS:H    | 6        | 0.12          |
| (1,1548) | 1:B:128:VAL:H   | 1:B:150:LYS:HD2 | 3        | 0.12          |
| (1,1548) | 1:B:128:VAL:H   | 1:B:150:LYS:HD3 | 3        | 0.12          |
| (1,1548) | 1:B:128:VAL:H   | 1:B:150:LYS:HD2 | 6        | 0.12          |
| (1,1548) | 1:B:128:VAL:H   | 1:B:150:LYS:HD3 | 6        | 0.12          |
| (1,1547) | 1:B:128:VAL:H   | 1:B:129:ASP:H   | 6        | 0.12          |
| (1,1529) | 1:B:127:ASP:H   | 1:B:125:PRO:HB2 | 2        | 0.12          |
| (1,1529) | 1:B:127:ASP:H   | 1:B:125:PRO:HB3 | 2        | 0.12          |
| (1,1528) | 1:B:126:ALA:HB1 | 1:B:128:VAL:H   | 2        | 0.12          |
| (1,1528) | 1:B:126:ALA:HB2 | 1:B:128:VAL:H   | 2        | 0.12          |
| (1,1528) | 1:B:126:ALA:HB3 | 1:B:128:VAL:H   | 2        | 0.12          |
| (1,1474) | 1:B:123:ARG:HB3 | 1:B:123:ARG:HD2 | 3        | 0.12          |
| (1,1474) | 1:B:123:ARG:HB3 | 1:B:123:ARG:HD3 | 3        | 0.12          |
| (1,1465) | 1:B:122:TYR:HB2 | 1:B:122:TYR:H   | 1        | 0.12          |
| (1,1465) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H   | 1        | 0.12          |
| (1,1464) | 1:B:122:TYR:HB2 | 1:B:122:TYR:H   | 1        | 0.12          |
| (1,1464) | 1:B:122:TYR:HB3 | 1:B:122:TYR:H   | 1        | 0.12          |
| (1,1463) | 1:B:122:TYR:HA  | 1:B:122:TYR:H   | 4        | 0.12          |
| (1,1456) | 1:B:122:TYR:HE1 | 1:B:98:ILE:HG21 | 8        | 0.12          |
| (1,1456) | 1:B:122:TYR:HE1 | 1:B:98:ILE:HG22 | 8        | 0.12          |
| (1,1456) | 1:B:122:TYR:HE1 | 1:B:98:ILE:HG23 | 8        | 0.12          |
| (1,1456) | 1:B:122:TYR:HE2 | 1:B:98:ILE:HG21 | 8        | 0.12          |
| (1,1456) | 1:B:122:TYR:HE2 | 1:B:98:ILE:HG22 | 8        | 0.12          |
| (1,1456) | 1:B:122:TYR:HE2 | 1:B:98:ILE:HG23 | 8        | 0.12          |
| (1,1426) | 1:B:118:PHE:HA  | 1:B:118:PHE:HD1 | 2        | 0.12          |
| (1,1426) | 1:B:118:PHE:HA  | 1:B:118:PHE:HD2 | 2        | 0.12          |
| (1,1399) | 1:B:115:SER:HB3 | 1:B:116:ARG:H   | 2        | 0.12          |
| (1,1366) | 1:B:113:PHE:HA  | 1:B:113:PHE:H   | 6        | 0.12          |
| (1,1314) | 1:B:109:ASP:H   | 1:B:109:ASP:HB2 | 3        | 0.12          |
| (1,1314) | 1:B:109:ASP:H   | 1:B:109:ASP:HB3 | 3        | 0.12          |
| (1,1309) | 1:B:108:GLN:HA  | 1:B:108:GLN:HB2 | 4        | 0.12          |
| (1,1309) | 1:B:108:GLN:HA  | 1:B:108:GLN:HB3 | 4        | 0.12          |
| (1,130)  | 1:A:78:ASN:HB2  | 1:A:79:LEU:H    | 3        | 0.12          |
| (1,130)  | 1:A:78:ASN:HB2  | 1:A:79:LEU:H    | 5        | 0.12          |
| (1,129)  | 1:A:78:ASN:HB3  | 1:A:79:LEU:H    | 5        | 0.12          |
| (1,1286) | 1:B:105:GLU:HA  | 1:B:116:ARG:H   | 8        | 0.12          |
| (1,1281) | 1:B:105:GLU:HG2 | 1:B:105:GLU:H   | 8        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1281) | 1:B:105:GLU:HG3 | 1:B:105:GLU:H   | 8        | 0.12          |
| (1,1262) | 1:B:103:LYS:HG2 | 1:B:103:LYS:H   | 7        | 0.12          |
| (1,1262) | 1:B:103:LYS:HG3 | 1:B:103:LYS:H   | 7        | 0.12          |
| (1,1257) | 1:B:102:GLY:HA2 | 1:B:103:LYS:H   | 6        | 0.12          |
| (1,1239) | 1:B:101:HIS:HA  | 1:B:101:HIS:HD2 | 1        | 0.12          |
| (1,1239) | 1:B:101:HIS:HA  | 1:B:101:HIS:HD2 | 2        | 0.12          |
| (1,123)  | 1:A:78:ASN:HB3  | 1:A:78:ASN:H    | 4        | 0.12          |
| (1,123)  | 1:A:78:ASN:HB3  | 1:A:78:ASN:H    | 5        | 0.12          |
| (1,1208) | 1:B:98:ILE:HB   | 1:B:99:GLU:H    | 7        | 0.12          |
| (1,1208) | 1:B:98:ILE:HB   | 1:B:99:GLU:H    | 9        | 0.12          |
| (1,1202) | 1:B:98:ILE:H    | 1:B:97:VAL:H    | 1        | 0.12          |
| (1,1202) | 1:B:98:ILE:H    | 1:B:97:VAL:H    | 3        | 0.12          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD11 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD12 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD13 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD21 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD22 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE1  | 1:A:70:LEU:HD23 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD11 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD12 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD13 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD21 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD22 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE2  | 1:A:70:LEU:HD23 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD11 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD12 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD13 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD21 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD22 | 8        | 0.12          |
| (1,12)   | 1:A:68:MET:HE3  | 1:A:70:LEU:HD23 | 8        | 0.12          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD11 | 6        | 0.12          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD12 | 6        | 0.12          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD13 | 6        | 0.12          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD21 | 6        | 0.12          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD22 | 6        | 0.12          |
| (1,1164) | 1:B:95:GLY:HA2  | 1:B:94:LEU:HD23 | 6        | 0.12          |
| (1,1147) | 1:B:92:LYS:H    | 1:B:100:VAL:HA  | 4        | 0.12          |
| (1,1135) | 1:B:91:VAL:H    | 1:B:91:VAL:HG21 | 2        | 0.12          |
| (1,1135) | 1:B:91:VAL:H    | 1:B:91:VAL:HG22 | 2        | 0.12          |
| (1,1135) | 1:B:91:VAL:H    | 1:B:91:VAL:HG23 | 2        | 0.12          |
| (1,1030) | 1:B:81:VAL:HG21 | 1:B:83:HIS:H    | 6        | 0.12          |
| (1,1030) | 1:B:81:VAL:HG22 | 1:B:83:HIS:H    | 6        | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1030) | 1:B:81:VAL:HG23  | 1:B:83:HIS:H    | 6        | 0.12          |
| (1,970)  | 1:B:77:VAL:H     | 1:B:78:ASN:H    | 9        | 0.11          |
| (1,944)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB3 | 2        | 0.11          |
| (1,944)  | 1:B:76:SER:HB2   | 1:B:146:ASP:HB3 | 6        | 0.11          |
| (1,924)  | 1:B:75:PHE:H     | 1:B:149:ARG:H   | 5        | 0.11          |
| (1,923)  | 1:B:75:PHE:HD1   | 1:B:148:PRO:HA  | 8        | 0.11          |
| (1,923)  | 1:B:75:PHE:HD2   | 1:B:148:PRO:HA  | 8        | 0.11          |
| (1,914)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HD1  | 9        | 0.11          |
| (1,914)  | 1:B:75:PHE:HA    | 1:B:75:PHE:HD2  | 9        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB2  | 1        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB3  | 1        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB2  | 2        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB3  | 2        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB2  | 3        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB3  | 3        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB2  | 4        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB3  | 4        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB2  | 6        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB3  | 6        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB2  | 9        | 0.11          |
| (1,903)  | 1:B:74:ARG:H     | 1:B:73:ASP:HB3  | 9        | 0.11          |
| (1,856)  | 1:A:150:LYS:H    | 1:A:149:ARG:H   | 3        | 0.11          |
| (1,847)  | 1:A:147:GLY:HA2  | 1:A:147:GLY:H   | 1        | 0.11          |
| (1,847)  | 1:A:147:GLY:HA2  | 1:A:147:GLY:H   | 6        | 0.11          |
| (1,847)  | 1:A:147:GLY:HA2  | 1:A:147:GLY:H   | 9        | 0.11          |
| (1,834)  | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 2        | 0.11          |
| (1,834)  | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 4        | 0.11          |
| (1,834)  | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 7        | 0.11          |
| (1,833)  | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 2        | 0.11          |
| (1,833)  | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 4        | 0.11          |
| (1,833)  | 1:A:146:ASP:HB3  | 1:A:146:ASP:HA  | 7        | 0.11          |
| (1,805)  | 1:A:144:THR:HG21 | 1:A:145:VAL:H   | 5        | 0.11          |
| (1,805)  | 1:A:144:THR:HG22 | 1:A:145:VAL:H   | 5        | 0.11          |
| (1,805)  | 1:A:144:THR:HG23 | 1:A:145:VAL:H   | 5        | 0.11          |
| (1,794)  | 1:A:144:THR:HG21 | 1:A:78:ASN:HA   | 3        | 0.11          |
| (1,794)  | 1:A:144:THR:HG22 | 1:A:78:ASN:HA   | 3        | 0.11          |
| (1,794)  | 1:A:144:THR:HG23 | 1:A:78:ASN:HA   | 3        | 0.11          |
| (1,784)  | 1:A:142:VAL:H    | 1:A:143:LEU:H   | 2        | 0.11          |
| (1,77)   | 1:A:76:SER:HB2   | 1:A:146:ASP:HB3 | 2        | 0.11          |
| (1,77)   | 1:A:76:SER:HB2   | 1:A:146:ASP:HB3 | 6        | 0.11          |
| (1,75)   | 1:A:76:SER:HB3   | 1:A:146:ASP:HB3 | 9        | 0.11          |
| (1,737)  | 1:A:135:SER:HA   | 1:A:136:SER:H   | 7        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,713) | 1:A:133:ILE:HD11 | 1:A:130:PRO:HB2  | 9        | 0.11          |
| (1,713) | 1:A:133:ILE:HD11 | 1:A:130:PRO:HB3  | 9        | 0.11          |
| (1,713) | 1:A:133:ILE:HD12 | 1:A:130:PRO:HB2  | 9        | 0.11          |
| (1,713) | 1:A:133:ILE:HD12 | 1:A:130:PRO:HB3  | 9        | 0.11          |
| (1,713) | 1:A:133:ILE:HD13 | 1:A:130:PRO:HB2  | 9        | 0.11          |
| (1,713) | 1:A:133:ILE:HD13 | 1:A:130:PRO:HB3  | 9        | 0.11          |
| (1,711) | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE1   | 4        | 0.11          |
| (1,711) | 1:A:133:ILE:HG21 | 1:A:75:PHE:HE2   | 4        | 0.11          |
| (1,711) | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE1   | 4        | 0.11          |
| (1,711) | 1:A:133:ILE:HG22 | 1:A:75:PHE:HE2   | 4        | 0.11          |
| (1,711) | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE1   | 4        | 0.11          |
| (1,711) | 1:A:133:ILE:HG23 | 1:A:75:PHE:HE2   | 4        | 0.11          |
| (1,700) | 1:A:132:THR:HG21 | 1:A:132:THR:H    | 2        | 0.11          |
| (1,700) | 1:A:132:THR:HG22 | 1:A:132:THR:H    | 2        | 0.11          |
| (1,700) | 1:A:132:THR:HG23 | 1:A:132:THR:H    | 2        | 0.11          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG11 | 4        | 0.11          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG12 | 4        | 0.11          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG13 | 4        | 0.11          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG21 | 4        | 0.11          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG22 | 4        | 0.11          |
| (1,674) | 1:A:127:ASP:H    | 1:A:128:VAL:HG23 | 4        | 0.11          |
| (1,661) | 1:A:126:ALA:HB1  | 1:A:128:VAL:H    | 2        | 0.11          |
| (1,661) | 1:A:126:ALA:HB2  | 1:A:128:VAL:H    | 2        | 0.11          |
| (1,661) | 1:A:126:ALA:HB3  | 1:A:128:VAL:H    | 2        | 0.11          |
| (1,656) | 1:A:125:PRO:HA   | 1:A:127:ASP:H    | 7        | 0.11          |
| (1,602) | 1:A:122:TYR:HA   | 1:A:123:ARG:H    | 6        | 0.11          |
| (1,589) | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG21  | 3        | 0.11          |
| (1,589) | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG22  | 3        | 0.11          |
| (1,589) | 1:A:122:TYR:HE1  | 1:A:98:ILE:HG23  | 3        | 0.11          |
| (1,589) | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG21  | 3        | 0.11          |
| (1,589) | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG22  | 3        | 0.11          |
| (1,589) | 1:A:122:TYR:HE2  | 1:A:98:ILE:HG23  | 3        | 0.11          |
| (1,57)  | 1:A:75:PHE:H     | 1:A:149:ARG:H    | 5        | 0.11          |
| (1,569) | 1:A:119:HIS:HA   | 1:A:101:HIS:HA   | 1        | 0.11          |
| (1,56)  | 1:A:75:PHE:HD1   | 1:A:148:PRO:HA   | 8        | 0.11          |
| (1,56)  | 1:A:75:PHE:HD2   | 1:A:148:PRO:HA   | 8        | 0.11          |
| (1,552) | 1:A:118:PHE:HE1  | 1:A:103:LYS:H    | 3        | 0.11          |
| (1,552) | 1:A:118:PHE:HE2  | 1:A:103:LYS:H    | 3        | 0.11          |
| (1,542) | 1:A:117:GLU:HA   | 1:A:103:LYS:HD2  | 5        | 0.11          |
| (1,542) | 1:A:117:GLU:HA   | 1:A:103:LYS:HD3  | 5        | 0.11          |
| (1,535) | 1:A:116:ARG:H    | 1:A:104:HIS:H    | 3        | 0.11          |
| (1,535) | 1:A:116:ARG:H    | 1:A:104:HIS:H    | 5        | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,534) | 1:A:116:ARG:H    | 1:A:104:HIS:H    | 3        | 0.11          |
| (1,534) | 1:A:116:ARG:H    | 1:A:104:HIS:H    | 5        | 0.11          |
| (1,532) | 1:A:115:SER:HB3  | 1:A:116:ARG:H    | 4        | 0.11          |
| (1,526) | 1:A:115:SER:HA   | 1:A:114:ILE:HD11 | 2        | 0.11          |
| (1,526) | 1:A:115:SER:HA   | 1:A:114:ILE:HD12 | 2        | 0.11          |
| (1,526) | 1:A:115:SER:HA   | 1:A:114:ILE:HD13 | 2        | 0.11          |
| (1,510) | 1:A:114:ILE:HG21 | 1:A:111:HIS:H    | 1        | 0.11          |
| (1,510) | 1:A:114:ILE:HG22 | 1:A:111:HIS:H    | 1        | 0.11          |
| (1,510) | 1:A:114:ILE:HG23 | 1:A:111:HIS:H    | 1        | 0.11          |
| (1,499) | 1:A:113:PHE:HA   | 1:A:113:PHE:H    | 6        | 0.11          |
| (1,482) | 1:A:113:PHE:HD1  | 1:A:107:ARG:HA   | 5        | 0.11          |
| (1,482) | 1:A:113:PHE:HD2  | 1:A:107:ARG:HA   | 5        | 0.11          |
| (1,47)  | 1:A:75:PHE:HA    | 1:A:75:PHE:HD1   | 9        | 0.11          |
| (1,47)  | 1:A:75:PHE:HA    | 1:A:75:PHE:HD2   | 9        | 0.11          |
| (1,442) | 1:A:108:GLN:HA   | 1:A:108:GLN:HB2  | 5        | 0.11          |
| (1,442) | 1:A:108:GLN:HA   | 1:A:108:GLN:HB3  | 5        | 0.11          |
| (1,425) | 1:A:107:ARG:HA   | 1:A:107:ARG:H    | 7        | 0.11          |
| (1,425) | 1:A:107:ARG:HA   | 1:A:107:ARG:H    | 9        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB2   | 1        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB3   | 1        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB2   | 2        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB3   | 2        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB2   | 3        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB3   | 3        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB2   | 4        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB3   | 4        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB2   | 6        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB3   | 6        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB2   | 9        | 0.11          |
| (1,36)  | 1:A:74:ARG:H     | 1:A:73:ASP:HB3   | 9        | 0.11          |
| (1,335) | 1:A:98:ILE:H     | 1:A:97:VAL:H     | 7        | 0.11          |
| (1,326) | 1:A:97:VAL:HB    | 1:A:97:VAL:HA    | 7        | 0.11          |
| (1,326) | 1:A:97:VAL:HB    | 1:A:97:VAL:HA    | 8        | 0.11          |
| (1,325) | 1:A:97:VAL:HB    | 1:A:97:VAL:HA    | 7        | 0.11          |
| (1,325) | 1:A:97:VAL:HB    | 1:A:97:VAL:HA    | 8        | 0.11          |
| (1,295) | 1:A:94:LEU:H     | 1:A:97:VAL:H     | 8        | 0.11          |
| (1,291) | 1:A:94:LEU:HD11  | 1:A:94:LEU:H     | 1        | 0.11          |
| (1,291) | 1:A:94:LEU:HD12  | 1:A:94:LEU:H     | 1        | 0.11          |
| (1,291) | 1:A:94:LEU:HD13  | 1:A:94:LEU:H     | 1        | 0.11          |
| (1,291) | 1:A:94:LEU:HD21  | 1:A:94:LEU:H     | 1        | 0.11          |
| (1,291) | 1:A:94:LEU:HD22  | 1:A:94:LEU:H     | 1        | 0.11          |
| (1,291) | 1:A:94:LEU:HD23  | 1:A:94:LEU:H     | 1        | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,288)  | 1:A:93:VAL:HA    | 1:A:99:GLU:H    | 8        | 0.11          |
| (1,279)  | 1:A:92:LYS:H     | 1:A:99:GLU:H    | 6        | 0.11          |
| (1,242)  | 1:A:89:LEU:H     | 1:A:88:GLU:H    | 6        | 0.11          |
| (1,241)  | 1:A:89:LEU:H     | 1:A:88:GLU:H    | 6        | 0.11          |
| (1,173)  | 1:A:83:HIS:HA    | 1:A:83:HIS:HD2  | 1        | 0.11          |
| (1,1723) | 1:B:150:LYS:H    | 1:B:149:ARG:H   | 3        | 0.11          |
| (1,1714) | 1:B:147:GLY:HA2  | 1:B:147:GLY:H   | 1        | 0.11          |
| (1,1714) | 1:B:147:GLY:HA2  | 1:B:147:GLY:H   | 6        | 0.11          |
| (1,1714) | 1:B:147:GLY:HA2  | 1:B:147:GLY:H   | 9        | 0.11          |
| (1,1701) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA  | 2        | 0.11          |
| (1,1701) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA  | 4        | 0.11          |
| (1,1701) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA  | 7        | 0.11          |
| (1,1700) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA  | 2        | 0.11          |
| (1,1700) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA  | 4        | 0.11          |
| (1,1700) | 1:B:146:ASP:HB3  | 1:B:146:ASP:HA  | 7        | 0.11          |
| (1,1672) | 1:B:144:THR:HG21 | 1:B:145:VAL:H   | 5        | 0.11          |
| (1,1672) | 1:B:144:THR:HG22 | 1:B:145:VAL:H   | 5        | 0.11          |
| (1,1672) | 1:B:144:THR:HG23 | 1:B:145:VAL:H   | 5        | 0.11          |
| (1,1651) | 1:B:142:VAL:H    | 1:B:143:LEU:H   | 2        | 0.11          |
| (1,1650) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1650) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1650) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1650) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1650) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1650) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1649) | 1:B:142:VAL:HG11 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1649) | 1:B:142:VAL:HG12 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1649) | 1:B:142:VAL:HG13 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1649) | 1:B:142:VAL:HG21 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1649) | 1:B:142:VAL:HG22 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1649) | 1:B:142:VAL:HG23 | 1:B:142:VAL:H   | 7        | 0.11          |
| (1,1604) | 1:B:135:SER:HA   | 1:B:136:SER:H   | 7        | 0.11          |
| (1,1580) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HB2 | 9        | 0.11          |
| (1,1580) | 1:B:133:ILE:HD11 | 1:B:130:PRO:HB3 | 9        | 0.11          |
| (1,1580) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HB2 | 9        | 0.11          |
| (1,1580) | 1:B:133:ILE:HD12 | 1:B:130:PRO:HB3 | 9        | 0.11          |
| (1,1580) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HB2 | 9        | 0.11          |
| (1,1580) | 1:B:133:ILE:HD13 | 1:B:130:PRO:HB3 | 9        | 0.11          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE1  | 4        | 0.11          |
| (1,1578) | 1:B:133:ILE:HG21 | 1:B:75:PHE:HE2  | 4        | 0.11          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE1  | 4        | 0.11          |
| (1,1578) | 1:B:133:ILE:HG22 | 1:B:75:PHE:HE2  | 4        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE1   | 4        | 0.11          |
| (1,1578) | 1:B:133:ILE:HG23 | 1:B:75:PHE:HE2   | 4        | 0.11          |
| (1,1572) | 1:B:132:THR:HG1  | 1:B:133:ILE:H    | 8        | 0.11          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG11 | 4        | 0.11          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG12 | 4        | 0.11          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG13 | 4        | 0.11          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG21 | 4        | 0.11          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG22 | 4        | 0.11          |
| (1,1541) | 1:B:127:ASP:H    | 1:B:128:VAL:HG23 | 4        | 0.11          |
| (1,1527) | 1:B:126:ALA:HA   | 1:B:128:VAL:H    | 1        | 0.11          |
| (1,1523) | 1:B:125:PRO:HA   | 1:B:127:ASP:H    | 7        | 0.11          |
| (1,1469) | 1:B:122:TYR:HA   | 1:B:123:ARG:H    | 6        | 0.11          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG21  | 3        | 0.11          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG22  | 3        | 0.11          |
| (1,1456) | 1:B:122:TYR:HE1  | 1:B:98:ILE:HG23  | 3        | 0.11          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG21  | 3        | 0.11          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG22  | 3        | 0.11          |
| (1,1456) | 1:B:122:TYR:HE2  | 1:B:98:ILE:HG23  | 3        | 0.11          |
| (1,1436) | 1:B:119:HIS:HA   | 1:B:101:HIS:HA   | 1        | 0.11          |
| (1,1419) | 1:B:118:PHE:HE1  | 1:B:103:LYS:H    | 3        | 0.11          |
| (1,1419) | 1:B:118:PHE:HE2  | 1:B:103:LYS:H    | 3        | 0.11          |
| (1,1409) | 1:B:117:GLU:HA   | 1:B:103:LYS:HD2  | 5        | 0.11          |
| (1,1409) | 1:B:117:GLU:HA   | 1:B:103:LYS:HD3  | 5        | 0.11          |
| (1,1402) | 1:B:116:ARG:H    | 1:B:104:HIS:H    | 3        | 0.11          |
| (1,1402) | 1:B:116:ARG:H    | 1:B:104:HIS:H    | 5        | 0.11          |
| (1,1401) | 1:B:116:ARG:H    | 1:B:104:HIS:H    | 3        | 0.11          |
| (1,1401) | 1:B:116:ARG:H    | 1:B:104:HIS:H    | 5        | 0.11          |
| (1,1399) | 1:B:115:SER:HB3  | 1:B:116:ARG:H    | 4        | 0.11          |
| (1,1399) | 1:B:115:SER:HB3  | 1:B:116:ARG:H    | 8        | 0.11          |
| (1,1377) | 1:B:114:ILE:HG21 | 1:B:111:HIS:H    | 1        | 0.11          |
| (1,1377) | 1:B:114:ILE:HG22 | 1:B:111:HIS:H    | 1        | 0.11          |
| (1,1377) | 1:B:114:ILE:HG23 | 1:B:111:HIS:H    | 1        | 0.11          |
| (1,1349) | 1:B:113:PHE:HD1  | 1:B:107:ARG:HA   | 5        | 0.11          |
| (1,1349) | 1:B:113:PHE:HD2  | 1:B:107:ARG:HA   | 5        | 0.11          |
| (1,1332) | 1:B:111:HIS:HB2  | 1:B:111:HIS:H    | 5        | 0.11          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB2  | 5        | 0.11          |
| (1,1309) | 1:B:108:GLN:HA   | 1:B:108:GLN:HB3  | 5        | 0.11          |
| (1,1294) | 1:B:107:ARG:HB3  | 1:B:107:ARG:H    | 5        | 0.11          |
| (1,1292) | 1:B:107:ARG:HA   | 1:B:107:ARG:H    | 7        | 0.11          |
| (1,1292) | 1:B:107:ARG:HA   | 1:B:107:ARG:H    | 9        | 0.11          |
| (1,1281) | 1:B:105:GLU:HG2  | 1:B:105:GLU:H    | 6        | 0.11          |
| (1,1281) | 1:B:105:GLU:HG3  | 1:B:105:GLU:H    | 6        | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1280) | 1:B:105:GLU:HG2 | 1:B:105:GLU:H  | 6        | 0.11          |
| (1,1280) | 1:B:105:GLU:HG3 | 1:B:105:GLU:H  | 6        | 0.11          |
| (1,1202) | 1:B:98:ILE:H    | 1:B:97:VAL:H   | 7        | 0.11          |
| (1,1193) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA  | 7        | 0.11          |
| (1,1193) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA  | 8        | 0.11          |
| (1,1192) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA  | 7        | 0.11          |
| (1,1192) | 1:B:97:VAL:HB   | 1:B:97:VAL:HA  | 8        | 0.11          |
| (1,1162) | 1:B:94:LEU:H    | 1:B:97:VAL:H   | 8        | 0.11          |
| (1,1158) | 1:B:94:LEU:HD11 | 1:B:94:LEU:H   | 1        | 0.11          |
| (1,1158) | 1:B:94:LEU:HD12 | 1:B:94:LEU:H   | 1        | 0.11          |
| (1,1158) | 1:B:94:LEU:HD13 | 1:B:94:LEU:H   | 1        | 0.11          |
| (1,1158) | 1:B:94:LEU:HD21 | 1:B:94:LEU:H   | 1        | 0.11          |
| (1,1158) | 1:B:94:LEU:HD22 | 1:B:94:LEU:H   | 1        | 0.11          |
| (1,1158) | 1:B:94:LEU:HD23 | 1:B:94:LEU:H   | 1        | 0.11          |
| (1,1155) | 1:B:93:VAL:HA   | 1:B:99:GLU:H   | 8        | 0.11          |
| (1,1146) | 1:B:92:LYS:H    | 1:B:99:GLU:H   | 6        | 0.11          |
| (1,1040) | 1:B:83:HIS:HA   | 1:B:83:HIS:HD2 | 1        | 0.11          |
| (1,103)  | 1:A:77:VAL:H    | 1:A:78:ASN:H   | 9        | 0.11          |

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

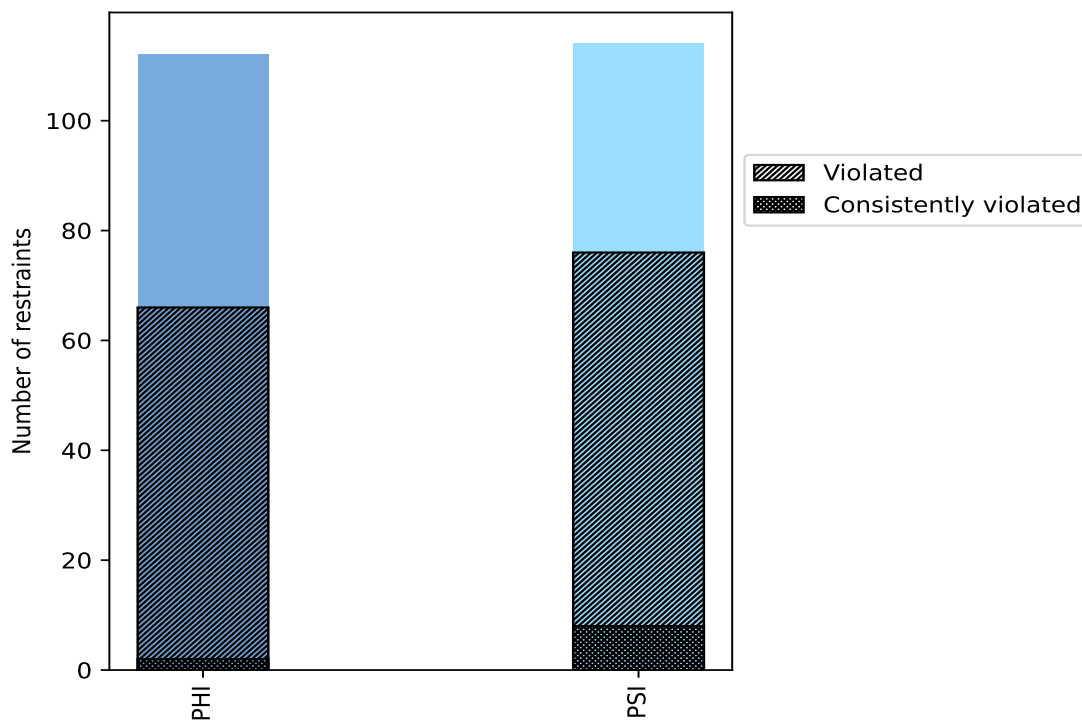
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 112   | 49.6           | 66                    | 58.9           | 29.2           | 2                                  | 1.8            | 0.9            |
| PSI        | 114   | 50.4           | 76                    | 66.7           | 33.6           | 8                                  | 7.0            | 3.5            |
| Total      | 226   | 100.0          | 142                   | 62.8           | 62.8           | 10                                 | 4.4            | 4.4            |

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

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



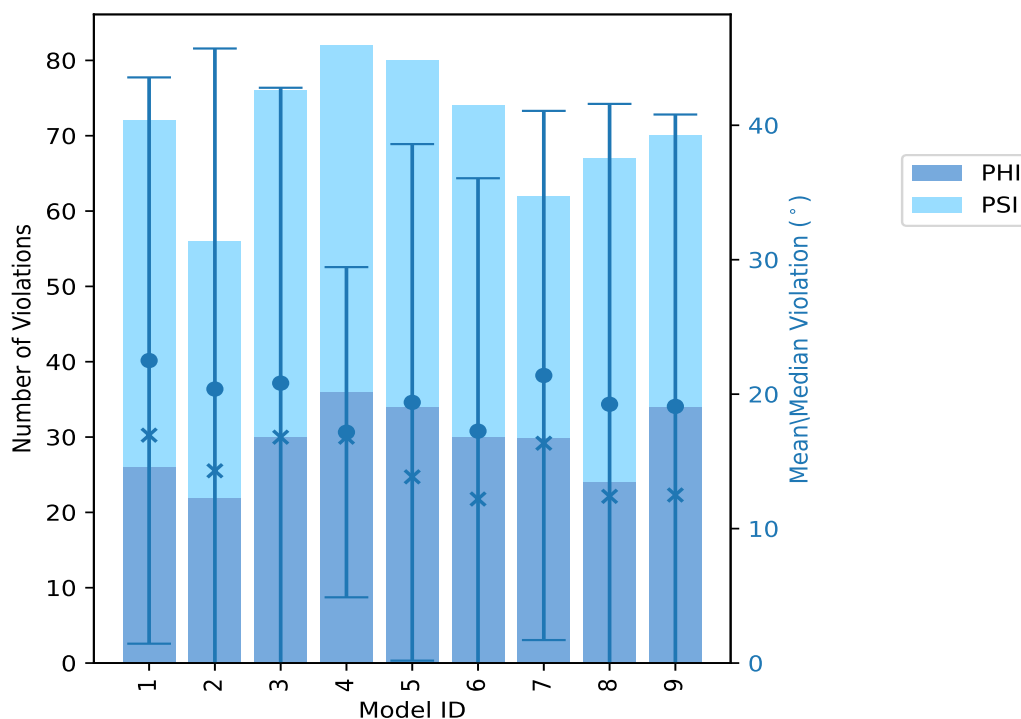
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 26                   | 46  | 72    | 22.5     | 108.8   | 21.06  | 16.95      |
| 2        | 22                   | 34  | 56    | 20.38    | 134.6   | 25.33  | 14.3       |
| 3        | 30                   | 46  | 76    | 20.82    | 118.0   | 21.97  | 16.8       |
| 4        | 36                   | 46  | 82    | 17.17    | 45.6    | 12.28  | 16.8       |
| 5        | 34                   | 46  | 80    | 19.39    | 107.5   | 19.21  | 13.85      |
| 6        | 30                   | 44  | 74    | 17.25    | 107.5   | 18.81  | 12.2       |
| 7        | 30                   | 32  | 62    | 21.39    | 105.0   | 19.68  | 16.35      |
| 8        | 24                   | 43  | 67    | 19.25    | 122.5   | 22.34  | 12.4       |
| 9        | 34                   | 36  | 70    | 19.09    | 119.6   | 21.71  | 12.5       |

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



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



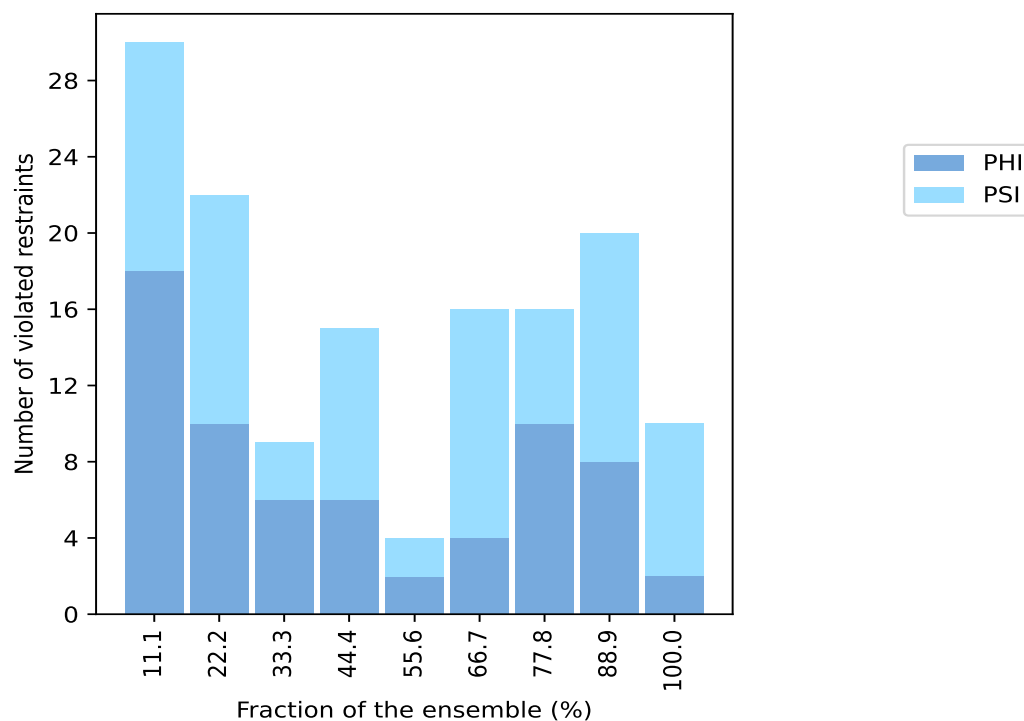
### 10.3 Dihedral-angle violation statistics for the ensemble [\(i\)](#)

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

| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |
| 18                            | 12  | 30    | 1                        | 11.1  |
| 10                            | 12  | 22    | 2                        | 22.2  |
| 6                             | 3   | 9     | 3                        | 33.3  |
| 6                             | 9   | 15    | 4                        | 44.4  |
| 2                             | 2   | 4     | 5                        | 55.6  |
| 4                             | 12  | 16    | 6                        | 66.7  |
| 10                            | 6   | 16    | 7                        | 77.8  |
| 8                             | 12  | 20    | 8                        | 88.9  |
| 2                             | 8   | 10    | 9                        | 100.0 |

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

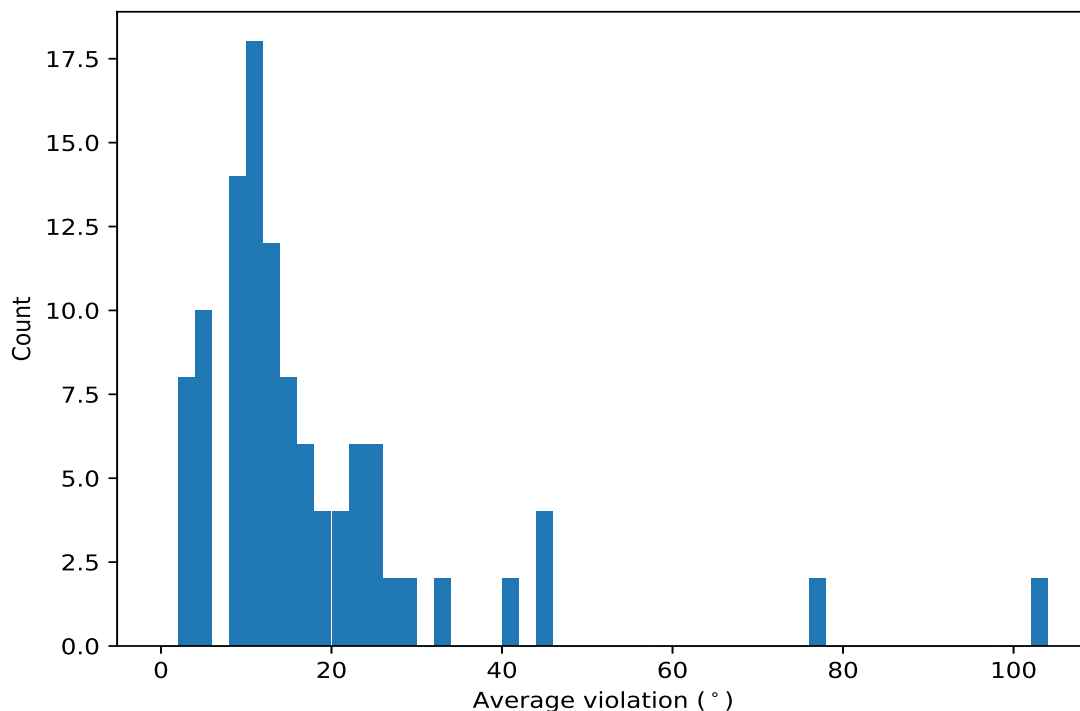
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [\(i\)](#)



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

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

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



### 10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean   | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|--------|-----------------|--------|
| (1,175) | 1:B:116:ARG:N | 1:B:116:ARG:CA | 1:B:116:ARG:C  | 1:B:117:GLU:N | 9                   | 32.91  | 20.4            | 34.9   |
| (1,62)  | 1:A:116:ARG:N | 1:A:116:ARG:CA | 1:A:116:ARG:C  | 1:A:117:GLU:N | 9                   | 32.87  | 20.38           | 34.7   |
| (1,28)  | 1:A:94:LEU:N  | 1:A:94:LEU:CA  | 1:A:94:LEU:C   | 1:A:95:GLY:N  | 9                   | 27.41  | 5.15            | 28.8   |
| (1,141) | 1:B:94:LEU:N  | 1:B:94:LEU:CA  | 1:B:94:LEU:C   | 1:B:95:GLY:N  | 9                   | 27.37  | 5.12            | 28.8   |
| (1,163) | 1:B:107:ARG:N | 1:B:107:ARG:CA | 1:B:107:ARG:C  | 1:B:108:GLN:N | 9                   | 23.78  | 10.39           | 23.3   |
| (1,50)  | 1:A:107:ARG:N | 1:A:107:ARG:CA | 1:A:107:ARG:C  | 1:A:108:GLN:N | 9                   | 23.69  | 10.38           | 23.4   |
| (1,32)  | 1:A:98:ILE:N  | 1:A:98:ILE:CA  | 1:A:98:ILE:C   | 1:A:99:GLU:N  | 9                   | 15.81  | 8.18            | 12.4   |
| (1,145) | 1:B:98:ILE:N  | 1:B:98:ILE:CA  | 1:B:98:ILE:C   | 1:B:99:GLU:N  | 9                   | 15.74  | 8.17            | 12.5   |
| (1,182) | 1:B:119:HIS:C | 1:B:120:ARG:N  | 1:B:120:ARG:CA | 1:B:120:ARG:C | 9                   | 13.27  | 6.36            | 15.5   |
| (1,69)  | 1:A:119:HIS:C | 1:A:120:ARG:N  | 1:A:120:ARG:CA | 1:A:120:ARG:C | 9                   | 13.24  | 6.38            | 15.5   |
| (1,47)  | 1:A:105:GLU:C | 1:A:106:GLU:N  | 1:A:106:GLU:CA | 1:A:106:GLU:C | 8                   | 102.78 | 26.86           | 108.1  |
| (1,160) | 1:B:105:GLU:C | 1:B:106:GLU:N  | 1:B:106:GLU:CA | 1:B:106:GLU:C | 8                   | 102.75 | 26.83           | 108.15 |
| (1,48)  | 1:A:106:GLU:N | 1:A:106:GLU:CA | 1:A:106:GLU:C  | 1:A:107:ARG:N | 8                   | 44.15  | 10.86           | 47.35  |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,161) | 1:B:106:GLU:N | 1:B:106:GLU:CA | 1:B:106:GLU:C  | 1:B:107:ARG:N | 8                   | 44.14 | 10.87           | 47.45  |
| (1,181) | 1:B:119:HIS:N | 1:B:119:HIS:CA | 1:B:119:HIS:C  | 1:B:120:ARG:N | 8                   | 29.8  | 7.94            | 32.4   |
| (1,68)  | 1:A:119:HIS:N | 1:A:119:HIS:CA | 1:A:119:HIS:C  | 1:A:120:ARG:N | 8                   | 29.79 | 7.96            | 32.5   |
| (1,60)  | 1:A:115:SER:N | 1:A:115:SER:CA | 1:A:115:SER:C  | 1:A:116:ARG:N | 8                   | 24.6  | 10.0            | 27.05  |
| (1,173) | 1:B:115:SER:N | 1:B:115:SER:CA | 1:B:115:SER:C  | 1:B:116:ARG:N | 8                   | 24.59 | 10.0            | 27.0   |
| (1,33)  | 1:A:98:ILE:C  | 1:A:99:GLU:N   | 1:A:99:GLU:CA  | 1:A:99:GLU:C  | 8                   | 24.4  | 8.34            | 23.0   |
| (1,146) | 1:B:98:ILE:C  | 1:B:99:GLU:N   | 1:B:99:GLU:CA  | 1:B:99:GLU:C  | 8                   | 24.38 | 8.37            | 22.95  |
| (1,149) | 1:B:100:VAL:N | 1:B:100:VAL:CA | 1:B:100:VAL:C  | 1:B:101:HIS:N | 8                   | 24.24 | 9.5             | 22.5   |
| (1,36)  | 1:A:100:VAL:N | 1:A:100:VAL:CA | 1:A:100:VAL:C  | 1:A:101:HIS:N | 8                   | 24.19 | 9.52            | 22.55  |
| (1,152) | 1:B:101:HIS:C | 1:B:102:GLY:N  | 1:B:102:GLY:CA | 1:B:102:GLY:C | 8                   | 23.18 | 11.97           | 22.75  |
| (1,39)  | 1:A:101:HIS:C | 1:A:102:GLY:N  | 1:A:102:GLY:CA | 1:A:102:GLY:C | 8                   | 23.14 | 11.94           | 22.8   |
| (1,139) | 1:B:93:VAL:N  | 1:B:93:VAL:CA  | 1:B:93:VAL:C   | 1:B:94:LEU:N  | 8                   | 21.86 | 6.47            | 24.5   |
| (1,26)  | 1:A:93:VAL:N  | 1:A:93:VAL:CA  | 1:A:93:VAL:C   | 1:A:94:LEU:N  | 8                   | 21.85 | 6.45            | 24.55  |
| (1,147) | 1:B:99:GLU:N  | 1:B:99:GLU:CA  | 1:B:99:GLU:C   | 1:B:100:VAL:N | 8                   | 16.3  | 7.3             | 15.6   |
| (1,34)  | 1:A:99:GLU:N  | 1:A:99:GLU:CA  | 1:A:99:GLU:C   | 1:A:100:VAL:N | 8                   | 16.25 | 7.33            | 15.5   |
| (1,63)  | 1:A:116:ARG:C | 1:A:117:GLU:N  | 1:A:117:GLU:CA | 1:A:117:GLU:C | 8                   | 13.39 | 11.0            | 10.1   |
| (1,176) | 1:B:116:ARG:C | 1:B:117:GLU:N  | 1:B:117:GLU:CA | 1:B:117:GLU:C | 8                   | 13.38 | 10.94           | 10.15  |
| (1,204) | 1:B:134:THR:N | 1:B:134:THR:CA | 1:B:134:THR:C  | 1:B:135:SER:N | 7                   | 20.13 | 17.44           | 10.6   |
| (1,91)  | 1:A:134:THR:N | 1:A:134:THR:CA | 1:A:134:THR:C  | 1:A:135:SER:N | 7                   | 20.11 | 17.39           | 10.6   |
| (1,24)  | 1:A:92:LYS:N  | 1:A:92:LYS:CA  | 1:A:92:LYS:C   | 1:A:93:VAL:N  | 7                   | 18.21 | 8.15            | 22.2   |
| (1,137) | 1:B:92:LYS:N  | 1:B:92:LYS:CA  | 1:B:92:LYS:C   | 1:B:93:VAL:N  | 7                   | 18.2  | 8.16            | 22.2   |
| (1,150) | 1:B:100:VAL:C | 1:B:101:HIS:N  | 1:B:101:HIS:CA | 1:B:101:HIS:C | 7                   | 17.06 | 9.13            | 14.2   |
| (1,37)  | 1:A:100:VAL:C | 1:A:101:HIS:N  | 1:A:101:HIS:CA | 1:A:101:HIS:C | 7                   | 16.99 | 9.08            | 14.3   |
| (1,58)  | 1:A:114:ILE:N | 1:A:114:ILE:CA | 1:A:114:ILE:C  | 1:A:115:SER:N | 7                   | 14.56 | 13.37           | 8.3    |
| (1,171) | 1:B:114:ILE:N | 1:B:114:ILE:CA | 1:B:114:ILE:C  | 1:B:115:SER:N | 7                   | 14.54 | 13.35           | 8.3    |
| (1,164) | 1:B:107:ARG:C | 1:B:108:GLN:N  | 1:B:108:GLN:CA | 1:B:108:GLN:C | 7                   | 12.63 | 7.72            | 8.3    |
| (1,51)  | 1:A:107:ARG:C | 1:A:108:GLN:N  | 1:A:108:GLN:CA | 1:A:108:GLN:C | 7                   | 12.6  | 7.6             | 8.4    |
| (1,41)  | 1:A:102:GLY:C | 1:A:103:LYS:N  | 1:A:103:LYS:CA | 1:A:103:LYS:C | 7                   | 11.69 | 4.23            | 10.6   |
| (1,154) | 1:B:102:GLY:C | 1:B:103:LYS:N  | 1:B:103:LYS:CA | 1:B:103:LYS:C | 7                   | 11.69 | 4.26            | 10.7   |
| (1,21)  | 1:A:90:LYS:C  | 1:A:91:VAL:N   | 1:A:91:VAL:CA  | 1:A:91:VAL:C  | 7                   | 10.84 | 5.65            | 9.6    |
| (1,134) | 1:B:90:LYS:C  | 1:B:91:VAL:N   | 1:B:91:VAL:CA  | 1:B:91:VAL:C  | 7                   | 10.84 | 5.71            | 9.6    |
| (1,35)  | 1:A:99:GLU:C  | 1:A:100:VAL:N  | 1:A:100:VAL:CA | 1:A:100:VAL:C | 7                   | 9.59  | 3.77            | 8.4    |
| (1,148) | 1:B:99:GLU:C  | 1:B:100:VAL:N  | 1:B:100:VAL:CA | 1:B:100:VAL:C | 7                   | 9.59  | 3.72            | 8.4    |
| (1,54)  | 1:A:111:HIS:N | 1:A:111:HIS:CA | 1:A:111:HIS:C  | 1:A:112:GLY:N | 6                   | 45.13 | 9.64            | 44.8   |
| (1,167) | 1:B:111:HIS:N | 1:B:111:HIS:CA | 1:B:111:HIS:C  | 1:B:112:GLY:N | 6                   | 45.02 | 9.65            | 44.65  |
| (1,151) | 1:B:101:HIS:N | 1:B:101:HIS:CA | 1:B:101:HIS:C  | 1:B:102:GLY:N | 6                   | 41.27 | 7.43            | 45.0   |
| (1,38)  | 1:A:101:HIS:N | 1:A:101:HIS:CA | 1:A:101:HIS:C  | 1:A:102:GLY:N | 6                   | 41.2  | 7.47            | 45.0   |
| (1,20)  | 1:A:90:LYS:N  | 1:A:90:LYS:CA  | 1:A:90:LYS:C   | 1:A:91:VAL:N  | 6                   | 22.48 | 13.64           | 21.2   |
| (1,133) | 1:B:90:LYS:N  | 1:B:90:LYS:CA  | 1:B:90:LYS:C   | 1:B:91:VAL:N  | 6                   | 22.47 | 13.64           | 21.15  |
| (1,113) | 1:A:146:ASP:N | 1:A:146:ASP:CA | 1:A:146:ASP:C  | 1:A:147:GLY:N | 6                   | 13.48 | 8.29            | 13.65  |
| (1,226) | 1:B:146:ASP:N | 1:B:146:ASP:CA | 1:B:146:ASP:C  | 1:B:147:GLY:N | 6                   | 13.48 | 8.32            | 13.65  |
| (1,174) | 1:B:115:SER:C | 1:B:116:ARG:N  | 1:B:116:ARG:CA | 1:B:116:ARG:C | 6                   | 11.03 | 14.09           | 6.05   |
| (1,61)  | 1:A:115:SER:C | 1:A:116:ARG:N  | 1:A:116:ARG:CA | 1:A:116:ARG:C | 6                   | 11.02 | 14.04           | 6.0    |
| (1,66)  | 1:A:118:PHE:N | 1:A:118:PHE:CA | 1:A:118:PHE:C  | 1:A:119:HIS:N | 6                   | 10.27 | 3.97            | 10.5   |
| (1,179) | 1:B:118:PHE:N | 1:B:118:PHE:CA | 1:B:118:PHE:C  | 1:B:119:HIS:N | 6                   | 10.25 | 3.96            | 10.5   |
| (1,25)  | 1:A:92:LYS:C  | 1:A:93:VAL:N   | 1:A:93:VAL:CA  | 1:A:93:VAL:C  | 6                   | 4.98  | 2.22            | 4.55   |
| (1,138) | 1:B:92:LYS:C  | 1:B:93:VAL:N   | 1:B:93:VAL:CA  | 1:B:93:VAL:C  | 6                   | 4.93  | 2.25            | 4.55   |
| (1,12)  | 1:A:80:ASP:N  | 1:A:80:ASP:CA  | 1:A:80:ASP:C   | 1:A:81:VAL:N  | 6                   | 4.5   | 3.48            | 2.75   |
| (1,125) | 1:B:80:ASP:N  | 1:B:80:ASP:CA  | 1:B:80:ASP:C   | 1:B:81:VAL:N  | 6                   | 4.48  | 3.41            | 2.75   |
| (1,18)  | 1:A:89:LEU:N  | 1:A:89:LEU:CA  | 1:A:89:LEU:C   | 1:A:90:LYS:N  | 5                   | 16.78 | 7.39            | 12.8   |
| (1,131) | 1:B:89:LEU:N  | 1:B:89:LEU:CA  | 1:B:89:LEU:C   | 1:B:90:LYS:N  | 5                   | 16.74 | 7.39            | 12.7   |

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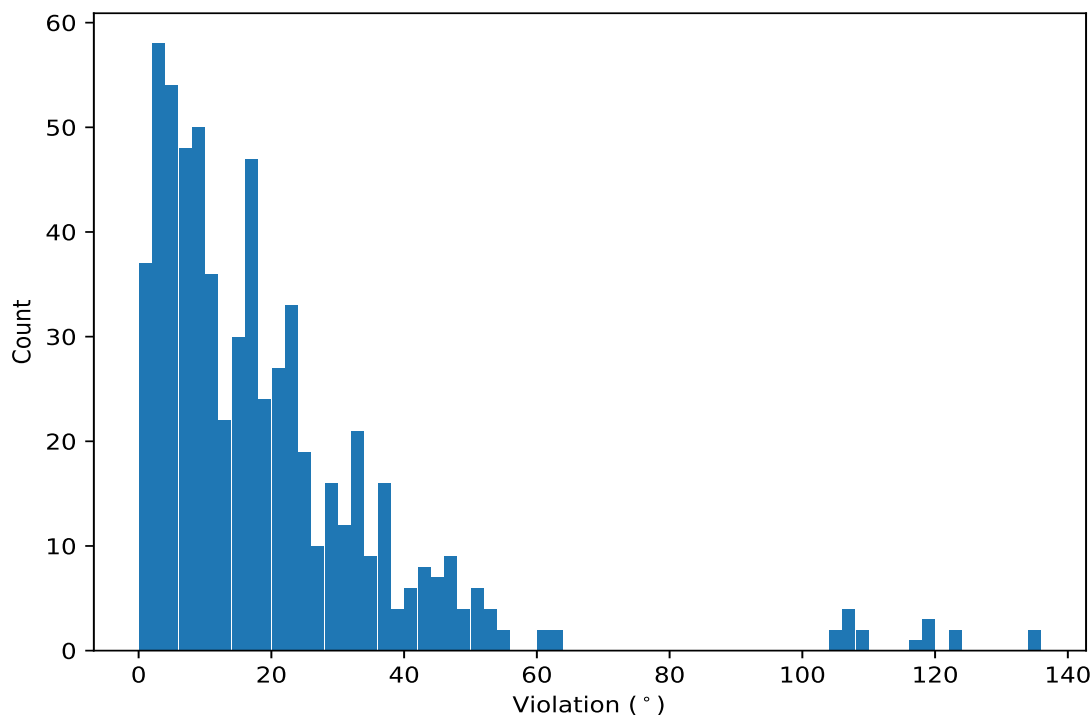
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,27)  | 1:A:93:VAL:C  | 1:A:94:LEU:N   | 1:A:94:LEU:CA  | 1:A:94:LEU:C  | 5                   | 3.72  | 2.1             | 4.0    |
| (1,140) | 1:B:93:VAL:C  | 1:B:94:LEU:N   | 1:B:94:LEU:CA  | 1:B:94:LEU:C  | 5                   | 3.7   | 2.18            | 4.0    |
| (1,53)  | 1:A:110:GLU:C | 1:A:111:HIS:N  | 1:A:111:HIS:CA | 1:A:111:HIS:C | 4                   | 14.97 | 5.6             | 16.35  |
| (1,166) | 1:B:110:GLU:C | 1:B:111:HIS:N  | 1:B:111:HIS:CA | 1:B:111:HIS:C | 4                   | 14.97 | 5.6             | 16.35  |
| (1,92)  | 1:A:134:THR:C | 1:A:135:SER:N  | 1:A:135:SER:CA | 1:A:135:SER:C | 4                   | 10.65 | 8.28            | 10.65  |
| (1,205) | 1:B:134:THR:C | 1:B:135:SER:N  | 1:B:135:SER:CA | 1:B:135:SER:C | 4                   | 10.63 | 8.25            | 10.65  |
| (1,6)   | 1:A:77:VAL:N  | 1:A:77:VAL:CA  | 1:A:77:VAL:C   | 1:A:78:ASN:N  | 4                   | 10.45 | 4.99            | 8.1    |
| (1,119) | 1:B:77:VAL:N  | 1:B:77:VAL:CA  | 1:B:77:VAL:C   | 1:B:78:ASN:N  | 4                   | 10.38 | 5.04            | 8.0    |
| (1,121) | 1:B:78:ASN:N  | 1:B:78:ASN:CA  | 1:B:78:ASN:C   | 1:B:79:LEU:N  | 4                   | 10.0  | 8.84            | 6.15   |
| (1,8)   | 1:A:78:ASN:N  | 1:A:78:ASN:CA  | 1:A:78:ASN:C   | 1:A:79:LEU:N  | 4                   | 9.98  | 8.8             | 6.15   |
| (1,70)  | 1:A:120:ARG:N | 1:A:120:ARG:CA | 1:A:120:ARG:C  | 1:A:121:LYS:N | 4                   | 8.1   | 4.42            | 6.9    |
| (1,183) | 1:B:120:ARG:N | 1:B:120:ARG:CA | 1:B:120:ARG:C  | 1:B:121:LYS:N | 4                   | 8.1   | 4.51            | 6.95   |
| (1,224) | 1:B:145:VAL:N | 1:B:145:VAL:CA | 1:B:145:VAL:C  | 1:B:146:ASP:N | 4                   | 8.02  | 5.33            | 8.15   |
| (1,72)  | 1:A:121:LYS:N | 1:A:121:LYS:CA | 1:A:121:LYS:C  | 1:A:122:TYR:N | 4                   | 5.82  | 0.94            | 6.3    |
| (1,185) | 1:B:121:LYS:N | 1:B:121:LYS:CA | 1:B:121:LYS:C  | 1:B:122:TYR:N | 4                   | 5.8   | 0.99            | 6.25   |
| (1,55)  | 1:A:112:GLY:C | 1:A:113:PHE:N  | 1:A:113:PHE:CA | 1:A:113:PHE:C | 4                   | 4.6   | 3.67            | 3.3    |
| (1,168) | 1:B:112:GLY:C | 1:B:113:PHE:N  | 1:B:113:PHE:CA | 1:B:113:PHE:C | 4                   | 4.58  | 3.56            | 3.3    |
| (1,67)  | 1:A:118:PHE:C | 1:A:119:HIS:N  | 1:A:119:HIS:CA | 1:A:119:HIS:C | 3                   | 11.87 | 7.06            | 16.3   |
| (1,180) | 1:B:118:PHE:C | 1:B:119:HIS:N  | 1:B:119:HIS:CA | 1:B:119:HIS:C | 3                   | 11.8  | 7.09            | 16.2   |
| (1,111) | 1:A:145:VAL:N | 1:A:145:VAL:CA | 1:A:145:VAL:C  | 1:A:146:ASP:N | 3                   | 10.4  | 4.12            | 11.5   |
| (1,73)  | 1:A:121:LYS:C | 1:A:122:TYR:N  | 1:A:122:TYR:CA | 1:A:122:TYR:C | 3                   | 8.7   | 5.4             | 9.8    |
| (1,186) | 1:B:121:LYS:C | 1:B:122:TYR:N  | 1:B:122:TYR:CA | 1:B:122:TYR:C | 3                   | 8.63  | 5.31            | 9.6    |
| (1,135) | 1:B:91:VAL:N  | 1:B:91:VAL:CA  | 1:B:91:VAL:C   | 1:B:92:LYS:N  | 3                   | 4.5   | 3.37            | 2.8    |
| (1,22)  | 1:A:91:VAL:N  | 1:A:91:VAL:CA  | 1:A:91:VAL:C   | 1:A:92:LYS:N  | 3                   | 4.47  | 3.4             | 2.8    |
| (1,11)  | 1:A:79:LEU:C  | 1:A:80:ASP:N   | 1:A:80:ASP:CA  | 1:A:80:ASP:C  | 3                   | 3.93  | 1.43            | 4.4    |
| (1,124) | 1:B:79:LEU:C  | 1:B:80:ASP:N   | 1:B:80:ASP:CA  | 1:B:80:ASP:C  | 3                   | 3.93  | 1.43            | 4.4    |
| (1,159) | 1:B:105:GLU:N | 1:B:105:GLU:CA | 1:B:105:GLU:C  | 1:B:106:GLU:N | 2                   | 76.25 | 58.35           | 76.25  |
| (1,46)  | 1:A:105:GLU:N | 1:A:105:GLU:CA | 1:A:105:GLU:C  | 1:A:106:GLU:N | 2                   | 76.2  | 58.2            | 76.2   |
| (1,105) | 1:A:142:VAL:N | 1:A:142:VAL:CA | 1:A:142:VAL:C  | 1:A:143:LEU:N | 2                   | 18.1  | 4.6             | 18.1   |
| (1,218) | 1:B:142:VAL:N | 1:B:142:VAL:CA | 1:B:142:VAL:C  | 1:B:143:LEU:N | 2                   | 18.1  | 4.7             | 18.1   |
| (1,17)  | 1:A:88:GLU:C  | 1:A:89:LEU:N   | 1:A:89:LEU:CA  | 1:A:89:LEU:C  | 2                   | 15.3  | 5.0             | 15.3   |
| (1,130) | 1:B:88:GLU:C  | 1:B:89:LEU:N   | 1:B:89:LEU:CA  | 1:B:89:LEU:C  | 2                   | 15.25 | 4.85            | 15.25  |
| (1,122) | 1:B:78:ASN:C  | 1:B:79:LEU:N   | 1:B:79:LEU:CA  | 1:B:79:LEU:C  | 2                   | 13.95 | 9.55            | 13.95  |
| (1,9)   | 1:A:78:ASN:C  | 1:A:79:LEU:N   | 1:A:79:LEU:CA  | 1:A:79:LEU:C  | 2                   | 13.9  | 9.6             | 13.9   |
| (1,85)  | 1:A:130:PRO:N | 1:A:130:PRO:CA | 1:A:130:PRO:C  | 1:A:131:LEU:N | 2                   | 13.9  | 6.6             | 13.9   |
| (1,198) | 1:B:130:PRO:N | 1:B:130:PRO:CA | 1:B:130:PRO:C  | 1:B:131:LEU:N | 2                   | 13.8  | 6.6             | 13.8   |
| (1,57)  | 1:A:113:PHE:C | 1:A:114:ILE:N  | 1:A:114:ILE:CA | 1:A:114:ILE:C | 2                   | 10.55 | 7.95            | 10.55  |
| (1,170) | 1:B:113:PHE:C | 1:B:114:ILE:N  | 1:B:114:ILE:CA | 1:B:114:ILE:C | 2                   | 10.5  | 8.0             | 10.5   |
| (1,222) | 1:B:144:THR:N | 1:B:144:THR:CA | 1:B:144:THR:C  | 1:B:145:VAL:N | 2                   | 8.8   | 5.6             | 8.8    |
| (1,109) | 1:A:144:THR:N | 1:A:144:THR:CA | 1:A:144:THR:C  | 1:A:145:VAL:N | 2                   | 8.65  | 5.65            | 8.65   |
| (1,4)   | 1:A:76:SER:N  | 1:A:76:SER:CA  | 1:A:76:SER:C   | 1:A:77:VAL:N  | 2                   | 8.2   | 4.3             | 8.2    |
| (1,40)  | 1:A:102:GLY:N | 1:A:102:GLY:CA | 1:A:102:GLY:C  | 1:A:103:LYS:N | 2                   | 8.2   | 1.0             | 8.2    |
| (1,117) | 1:B:76:SER:N  | 1:B:76:SER:CA  | 1:B:76:SER:C   | 1:B:77:VAL:N  | 2                   | 8.2   | 4.3             | 8.2    |
| (1,153) | 1:B:102:GLY:N | 1:B:102:GLY:CA | 1:B:102:GLY:C  | 1:B:103:LYS:N | 2                   | 8.2   | 0.9             | 8.2    |
| (1,116) | 1:B:75:PHE:C  | 1:B:76:SER:N   | 1:B:76:SER:CA  | 1:B:76:SER:C  | 2                   | 2.85  | 1.05            | 2.85   |
| (1,3)   | 1:A:75:PHE:C  | 1:A:76:SER:N   | 1:A:76:SER:CA  | 1:A:76:SER:C  | 2                   | 2.8   | 1.0             | 2.8    |
| (1,5)   | 1:A:76:SER:C  | 1:A:77:VAL:N   | 1:A:77:VAL:CA  | 1:A:77:VAL:C  | 2                   | 2.1   | 0.3             | 2.1    |
| (1,118) | 1:B:76:SER:C  | 1:B:77:VAL:N   | 1:B:77:VAL:CA  | 1:B:77:VAL:C  | 2                   | 2.1   | 0.4             | 2.1    |

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

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

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

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,159) | 1:B:105:GLU:N | 1:B:105:GLU:CA | 1:B:105:GLU:C  | 1:B:106:GLU:N | 2        | 134.6         |
| (1,46)  | 1:A:105:GLU:N | 1:A:105:GLU:CA | 1:A:105:GLU:C  | 1:A:106:GLU:N | 2        | 134.4         |
| (1,47)  | 1:A:105:GLU:C | 1:A:106:GLU:N  | 1:A:106:GLU:CA | 1:A:106:GLU:C | 8        | 122.5         |
| (1,160) | 1:B:105:GLU:C | 1:B:106:GLU:N  | 1:B:106:GLU:CA | 1:B:106:GLU:C | 8        | 122.2         |
| (1,160) | 1:B:105:GLU:C | 1:B:106:GLU:N  | 1:B:106:GLU:CA | 1:B:106:GLU:C | 9        | 119.6         |
| (1,47)  | 1:A:105:GLU:C | 1:A:106:GLU:N  | 1:A:106:GLU:CA | 1:A:106:GLU:C | 9        | 119.5         |
| (1,47)  | 1:A:105:GLU:C | 1:A:106:GLU:N  | 1:A:106:GLU:CA | 1:A:106:GLU:C | 3        | 118.0         |
| (1,160) | 1:B:105:GLU:C | 1:B:106:GLU:N  | 1:B:106:GLU:CA | 1:B:106:GLU:C | 3        | 117.9         |
| (1,47)  | 1:A:105:GLU:C | 1:A:106:GLU:N  | 1:A:106:GLU:CA | 1:A:106:GLU:C | 1        | 108.8         |
| (1,160) | 1:B:105:GLU:C | 1:B:106:GLU:N  | 1:B:106:GLU:CA | 1:B:106:GLU:C | 1        | 108.8         |
| (1,160) | 1:B:105:GLU:C | 1:B:106:GLU:N  | 1:B:106:GLU:CA | 1:B:106:GLU:C | 5        | 107.5         |
| (1,160) | 1:B:105:GLU:C | 1:B:106:GLU:N  | 1:B:106:GLU:CA | 1:B:106:GLU:C | 6        | 107.5         |
| (1,47)  | 1:A:105:GLU:C | 1:A:106:GLU:N  | 1:A:106:GLU:CA | 1:A:106:GLU:C | 5        | 107.4         |
| (1,47)  | 1:A:105:GLU:C | 1:A:106:GLU:N  | 1:A:106:GLU:CA | 1:A:106:GLU:C | 6        | 107.4         |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,47)  | 1:A:105:GLU:C | 1:A:106:GLU:N  | 1:A:106:GLU:CA | 1:A:106:GLU:C | 7        | 105.0         |
| (1,160) | 1:B:105:GLU:C | 1:B:106:GLU:N  | 1:B:106:GLU:CA | 1:B:106:GLU:C | 7        | 104.9         |
| (1,175) | 1:B:116:ARG:N | 1:B:116:ARG:CA | 1:B:116:ARG:C  | 1:B:117:GLU:N | 3        | 63.6          |
| (1,62)  | 1:A:116:ARG:N | 1:A:116:ARG:CA | 1:A:116:ARG:C  | 1:A:117:GLU:N | 3        | 63.5          |
| (1,54)  | 1:A:111:HIS:N | 1:A:111:HIS:CA | 1:A:111:HIS:C  | 1:A:112:GLY:N | 1        | 60.5          |
| (1,167) | 1:B:111:HIS:N | 1:B:111:HIS:CA | 1:B:111:HIS:C  | 1:B:112:GLY:N | 1        | 60.4          |
| (1,62)  | 1:A:116:ARG:N | 1:A:116:ARG:CA | 1:A:116:ARG:C  | 1:A:117:GLU:N | 1        | 55.0          |
| (1,175) | 1:B:116:ARG:N | 1:B:116:ARG:CA | 1:B:116:ARG:C  | 1:B:117:GLU:N | 1        | 55.0          |
| (1,48)  | 1:A:106:GLU:N | 1:A:106:GLU:CA | 1:A:106:GLU:C  | 1:A:107:ARG:N | 5        | 53.6          |
| (1,161) | 1:B:106:GLU:N | 1:B:106:GLU:CA | 1:B:106:GLU:C  | 1:B:107:ARG:N | 5        | 53.4          |
| (1,54)  | 1:A:111:HIS:N | 1:A:111:HIS:CA | 1:A:111:HIS:C  | 1:A:112:GLY:N | 2        | 53.1          |
| (1,167) | 1:B:111:HIS:N | 1:B:111:HIS:CA | 1:B:111:HIS:C  | 1:B:112:GLY:N | 2        | 53.0          |
| (1,62)  | 1:A:116:ARG:N | 1:A:116:ARG:CA | 1:A:116:ARG:C  | 1:A:117:GLU:N | 5        | 50.9          |
| (1,175) | 1:B:116:ARG:N | 1:B:116:ARG:CA | 1:B:116:ARG:C  | 1:B:117:GLU:N | 5        | 50.9          |
| (1,48)  | 1:A:106:GLU:N | 1:A:106:GLU:CA | 1:A:106:GLU:C  | 1:A:107:ARG:N | 8        | 50.4          |
| (1,161) | 1:B:106:GLU:N | 1:B:106:GLU:CA | 1:B:106:GLU:C  | 1:B:107:ARG:N | 8        | 50.2          |
| (1,91)  | 1:A:134:THR:N | 1:A:134:THR:CA | 1:A:134:THR:C  | 1:A:135:SER:N | 2        | 50.0          |
| (1,204) | 1:B:134:THR:N | 1:B:134:THR:CA | 1:B:134:THR:C  | 1:B:135:SER:N | 2        | 50.0          |
| (1,161) | 1:B:106:GLU:N | 1:B:106:GLU:CA | 1:B:106:GLU:C  | 1:B:107:ARG:N | 9        | 49.7          |
| (1,48)  | 1:A:106:GLU:N | 1:A:106:GLU:CA | 1:A:106:GLU:C  | 1:A:107:ARG:N | 9        | 49.6          |
| (1,161) | 1:B:106:GLU:N | 1:B:106:GLU:CA | 1:B:106:GLU:C  | 1:B:107:ARG:N | 3        | 48.9          |
| (1,48)  | 1:A:106:GLU:N | 1:A:106:GLU:CA | 1:A:106:GLU:C  | 1:A:107:ARG:N | 3        | 48.8          |
| (1,20)  | 1:A:90:LYS:N  | 1:A:90:LYS:CA  | 1:A:90:LYS:C   | 1:A:91:VAL:N  | 7        | 47.7          |
| (1,133) | 1:B:90:LYS:N  | 1:B:90:LYS:CA  | 1:B:90:LYS:C   | 1:B:91:VAL:N  | 7        | 47.7          |
| (1,151) | 1:B:101:HIS:N | 1:B:101:HIS:CA | 1:B:101:HIS:C  | 1:B:102:GLY:N | 5        | 47.2          |
| (1,38)  | 1:A:101:HIS:N | 1:A:101:HIS:CA | 1:A:101:HIS:C  | 1:A:102:GLY:N | 3        | 47.1          |
| (1,38)  | 1:A:101:HIS:N | 1:A:101:HIS:CA | 1:A:101:HIS:C  | 1:A:102:GLY:N | 5        | 47.1          |
| (1,151) | 1:B:101:HIS:N | 1:B:101:HIS:CA | 1:B:101:HIS:C  | 1:B:102:GLY:N | 3        | 47.1          |
| (1,38)  | 1:A:101:HIS:N | 1:A:101:HIS:CA | 1:A:101:HIS:C  | 1:A:102:GLY:N | 8        | 47.0          |
| (1,151) | 1:B:101:HIS:N | 1:B:101:HIS:CA | 1:B:101:HIS:C  | 1:B:102:GLY:N | 8        | 47.0          |
| (1,161) | 1:B:106:GLU:N | 1:B:106:GLU:CA | 1:B:106:GLU:C  | 1:B:107:ARG:N | 6        | 46.0          |
| (1,48)  | 1:A:106:GLU:N | 1:A:106:GLU:CA | 1:A:106:GLU:C  | 1:A:107:ARG:N | 6        | 45.9          |
| (1,54)  | 1:A:111:HIS:N | 1:A:111:HIS:CA | 1:A:111:HIS:C  | 1:A:112:GLY:N | 4        | 45.6          |
| (1,167) | 1:B:111:HIS:N | 1:B:111:HIS:CA | 1:B:111:HIS:C  | 1:B:112:GLY:N | 4        | 45.5          |
| (1,48)  | 1:A:106:GLU:N | 1:A:106:GLU:CA | 1:A:106:GLU:C  | 1:A:107:ARG:N | 7        | 45.2          |
| (1,161) | 1:B:106:GLU:N | 1:B:106:GLU:CA | 1:B:106:GLU:C  | 1:B:107:ARG:N | 7        | 45.2          |
| (1,204) | 1:B:134:THR:N | 1:B:134:THR:CA | 1:B:134:THR:C  | 1:B:135:SER:N | 3        | 44.1          |
| (1,54)  | 1:A:111:HIS:N | 1:A:111:HIS:CA | 1:A:111:HIS:C  | 1:A:112:GLY:N | 8        | 44.0          |
| (1,91)  | 1:A:134:THR:N | 1:A:134:THR:CA | 1:A:134:THR:C  | 1:A:135:SER:N | 3        | 43.9          |
| (1,167) | 1:B:111:HIS:N | 1:B:111:HIS:CA | 1:B:111:HIS:C  | 1:B:112:GLY:N | 8        | 43.8          |
| (1,161) | 1:B:106:GLU:N | 1:B:106:GLU:CA | 1:B:106:GLU:C  | 1:B:107:ARG:N | 1        | 43.2          |
| (1,48)  | 1:A:106:GLU:N | 1:A:106:GLU:CA | 1:A:106:GLU:C  | 1:A:107:ARG:N | 1        | 43.1          |
| (1,38)  | 1:A:101:HIS:N | 1:A:101:HIS:CA | 1:A:101:HIS:C  | 1:A:102:GLY:N | 6        | 43.0          |
| (1,151) | 1:B:101:HIS:N | 1:B:101:HIS:CA | 1:B:101:HIS:C  | 1:B:102:GLY:N | 6        | 43.0          |
| (1,174) | 1:B:115:SER:C | 1:B:116:ARG:N  | 1:B:116:ARG:CA | 1:B:116:ARG:C | 9        | 42.1          |
| (1,61)  | 1:A:115:SER:C | 1:A:116:ARG:N  | 1:A:116:ARG:CA | 1:A:116:ARG:C | 9        | 42.0          |
| (1,152) | 1:B:101:HIS:C | 1:B:102:GLY:N  | 1:B:102:GLY:CA | 1:B:102:GLY:C | 1        | 41.7          |
| (1,39)  | 1:A:101:HIS:C | 1:A:102:GLY:N  | 1:A:102:GLY:CA | 1:A:102:GLY:C | 1        | 41.5          |
| (1,60)  | 1:A:115:SER:N | 1:A:115:SER:CA | 1:A:115:SER:C  | 1:A:116:ARG:N | 9        | 41.0          |
| (1,33)  | 1:A:98:ILE:C  | 1:A:99:GLU:N   | 1:A:99:GLU:CA  | 1:A:99:GLU:C  | 9        | 40.9          |
| (1,173) | 1:B:115:SER:N | 1:B:115:SER:CA | 1:B:115:SER:C  | 1:B:116:ARG:N | 9        | 40.9          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,146) | 1:B:98:ILE:C  | 1:B:99:GLU:N   | 1:B:99:GLU:CA  | 1:B:99:GLU:C  | 9        | 40.9          |
| (1,163) | 1:B:107:ARG:N | 1:B:107:ARG:CA | 1:B:107:ARG:C  | 1:B:108:GLN:N | 4        | 39.6          |
| (1,50)  | 1:A:107:ARG:N | 1:A:107:ARG:CA | 1:A:107:ARG:C  | 1:A:108:GLN:N | 4        | 39.4          |
| (1,149) | 1:B:100:VAL:N | 1:B:100:VAL:CA | 1:B:100:VAL:C  | 1:B:101:HIS:N | 1        | 39.1          |
| (1,36)  | 1:A:100:VAL:N | 1:A:100:VAL:CA | 1:A:100:VAL:C  | 1:A:101:HIS:N | 1        | 39.0          |
| (1,68)  | 1:A:119:HIS:N | 1:A:119:HIS:CA | 1:A:119:HIS:C  | 1:A:120:ARG:N | 3        | 37.6          |
| (1,68)  | 1:A:119:HIS:N | 1:A:119:HIS:CA | 1:A:119:HIS:C  | 1:A:120:ARG:N | 7        | 37.6          |
| (1,181) | 1:B:119:HIS:N | 1:B:119:HIS:CA | 1:B:119:HIS:C  | 1:B:120:ARG:N | 3        | 37.6          |
| (1,150) | 1:B:100:VAL:C | 1:B:101:HIS:N  | 1:B:101:HIS:CA | 1:B:101:HIS:C | 1        | 37.6          |
| (1,37)  | 1:A:100:VAL:C | 1:A:101:HIS:N  | 1:A:101:HIS:CA | 1:A:101:HIS:C | 1        | 37.5          |
| (1,181) | 1:B:119:HIS:N | 1:B:119:HIS:CA | 1:B:119:HIS:C  | 1:B:120:ARG:N | 7        | 37.5          |
| (1,62)  | 1:A:116:ARG:N | 1:A:116:ARG:CA | 1:A:116:ARG:C  | 1:A:117:GLU:N | 6        | 36.8          |
| (1,175) | 1:B:116:ARG:N | 1:B:116:ARG:CA | 1:B:116:ARG:C  | 1:B:117:GLU:N | 6        | 36.8          |
| (1,58)  | 1:A:114:ILE:N | 1:A:114:ILE:CA | 1:A:114:ILE:C  | 1:A:115:SER:N | 1        | 36.5          |
| (1,171) | 1:B:114:ILE:N | 1:B:114:ILE:CA | 1:B:114:ILE:C  | 1:B:115:SER:N | 1        | 36.5          |
| (1,181) | 1:B:119:HIS:N | 1:B:119:HIS:CA | 1:B:119:HIS:C  | 1:B:120:ARG:N | 8        | 36.2          |
| (1,151) | 1:B:101:HIS:N | 1:B:101:HIS:CA | 1:B:101:HIS:C  | 1:B:102:GLY:N | 1        | 36.2          |
| (1,32)  | 1:A:98:ILE:N  | 1:A:98:ILE:CA  | 1:A:98:ILE:C   | 1:A:99:GLU:N  | 9        | 36.1          |
| (1,145) | 1:B:98:ILE:N  | 1:B:98:ILE:CA  | 1:B:98:ILE:C   | 1:B:99:GLU:N  | 9        | 36.1          |
| (1,68)  | 1:A:119:HIS:N | 1:A:119:HIS:CA | 1:A:119:HIS:C  | 1:A:120:ARG:N | 8        | 36.0          |
| (1,38)  | 1:A:101:HIS:N | 1:A:101:HIS:CA | 1:A:101:HIS:C  | 1:A:102:GLY:N | 1        | 36.0          |
| (1,152) | 1:B:101:HIS:C | 1:B:102:GLY:N  | 1:B:102:GLY:CA | 1:B:102:GLY:C | 4        | 35.4          |
| (1,39)  | 1:A:101:HIS:C | 1:A:102:GLY:N  | 1:A:102:GLY:CA | 1:A:102:GLY:C | 4        | 35.3          |
| (1,175) | 1:B:116:ARG:N | 1:B:116:ARG:CA | 1:B:116:ARG:C  | 1:B:117:GLU:N | 4        | 34.9          |
| (1,63)  | 1:A:116:ARG:C | 1:A:117:GLU:N  | 1:A:117:GLU:CA | 1:A:117:GLU:C | 3        | 34.7          |
| (1,62)  | 1:A:116:ARG:N | 1:A:116:ARG:CA | 1:A:116:ARG:C  | 1:A:117:GLU:N | 4        | 34.7          |
| (1,176) | 1:B:116:ARG:C | 1:B:117:GLU:N  | 1:B:117:GLU:CA | 1:B:117:GLU:C | 3        | 34.5          |
| (1,149) | 1:B:100:VAL:N | 1:B:100:VAL:CA | 1:B:100:VAL:C  | 1:B:101:HIS:N | 4        | 34.4          |
| (1,36)  | 1:A:100:VAL:N | 1:A:100:VAL:CA | 1:A:100:VAL:C  | 1:A:101:HIS:N | 4        | 34.3          |
| (1,54)  | 1:A:111:HIS:N | 1:A:111:HIS:CA | 1:A:111:HIS:C  | 1:A:112:GLY:N | 7        | 34.0          |
| (1,167) | 1:B:111:HIS:N | 1:B:111:HIS:CA | 1:B:111:HIS:C  | 1:B:112:GLY:N | 7        | 33.8          |
| (1,54)  | 1:A:111:HIS:N | 1:A:111:HIS:CA | 1:A:111:HIS:C  | 1:A:112:GLY:N | 5        | 33.6          |
| (1,47)  | 1:A:105:GLU:C | 1:A:106:GLU:N  | 1:A:106:GLU:CA | 1:A:106:GLU:C | 4        | 33.6          |
| (1,167) | 1:B:111:HIS:N | 1:B:111:HIS:CA | 1:B:111:HIS:C  | 1:B:112:GLY:N | 5        | 33.6          |
| (1,160) | 1:B:105:GLU:C | 1:B:106:GLU:N  | 1:B:106:GLU:CA | 1:B:106:GLU:C | 4        | 33.6          |
| (1,146) | 1:B:98:ILE:C  | 1:B:99:GLU:N   | 1:B:99:GLU:CA  | 1:B:99:GLU:C  | 8        | 33.4          |
| (1,33)  | 1:A:98:ILE:C  | 1:A:99:GLU:N   | 1:A:99:GLU:CA  | 1:A:99:GLU:C  | 8        | 33.3          |
| (1,28)  | 1:A:94:LEU:N  | 1:A:94:LEU:CA  | 1:A:94:LEU:C   | 1:A:95:GLY:N  | 5        | 33.0          |
| (1,141) | 1:B:94:LEU:N  | 1:B:94:LEU:CA  | 1:B:94:LEU:C   | 1:B:95:GLY:N  | 5        | 32.8          |
| (1,58)  | 1:A:114:ILE:N | 1:A:114:ILE:CA | 1:A:114:ILE:C  | 1:A:115:SER:N | 4        | 32.7          |
| (1,171) | 1:B:114:ILE:N | 1:B:114:ILE:CA | 1:B:114:ILE:C  | 1:B:115:SER:N | 4        | 32.6          |
| (1,68)  | 1:A:119:HIS:N | 1:A:119:HIS:CA | 1:A:119:HIS:C  | 1:A:120:ARG:N | 1        | 32.5          |
| (1,68)  | 1:A:119:HIS:N | 1:A:119:HIS:CA | 1:A:119:HIS:C  | 1:A:120:ARG:N | 5        | 32.5          |
| (1,28)  | 1:A:94:LEU:N  | 1:A:94:LEU:CA  | 1:A:94:LEU:C   | 1:A:95:GLY:N  | 3        | 32.4          |
| (1,181) | 1:B:119:HIS:N | 1:B:119:HIS:CA | 1:B:119:HIS:C  | 1:B:120:ARG:N | 1        | 32.4          |
| (1,181) | 1:B:119:HIS:N | 1:B:119:HIS:CA | 1:B:119:HIS:C  | 1:B:120:ARG:N | 5        | 32.4          |
| (1,173) | 1:B:115:SER:N | 1:B:115:SER:CA | 1:B:115:SER:C  | 1:B:116:ARG:N | 3        | 32.3          |
| (1,60)  | 1:A:115:SER:N | 1:A:115:SER:CA | 1:A:115:SER:C  | 1:A:116:ARG:N | 3        | 32.2          |
| (1,141) | 1:B:94:LEU:N  | 1:B:94:LEU:CA  | 1:B:94:LEU:C   | 1:B:95:GLY:N  | 3        | 32.2          |
| (1,39)  | 1:A:101:HIS:C | 1:A:102:GLY:N  | 1:A:102:GLY:CA | 1:A:102:GLY:C | 3        | 32.1          |
| (1,152) | 1:B:101:HIS:C | 1:B:102:GLY:N  | 1:B:102:GLY:CA | 1:B:102:GLY:C | 3        | 32.1          |

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| Key     | Atom-1        | Atom-2         | Atom-3        | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,163) | 1:B:107:ARG:N | 1:B:107:ARG:CA | 1:B:107:ARG:C | 1:B:108:GLN:N | 7        | 31.9          |
| (1,50)  | 1:A:107:ARG:N | 1:A:107:ARG:CA | 1:A:107:ARG:C | 1:A:108:GLN:N | 7        | 31.7          |
| (1,36)  | 1:A:100:VAL:N | 1:A:100:VAL:CA | 1:A:100:VAL:C | 1:A:101:HIS:N | 7        | 31.7          |
| (1,163) | 1:B:107:ARG:N | 1:B:107:ARG:CA | 1:B:107:ARG:C | 1:B:108:GLN:N | 5        | 31.7          |
| (1,50)  | 1:A:107:ARG:N | 1:A:107:ARG:CA | 1:A:107:ARG:C | 1:A:108:GLN:N | 5        | 31.6          |
| (1,149) | 1:B:100:VAL:N | 1:B:100:VAL:CA | 1:B:100:VAL:C | 1:B:101:HIS:N | 7        | 31.6          |
| (1,28)  | 1:A:94:LEU:N  | 1:A:94:LEU:CA  | 1:A:94:LEU:C  | 1:A:95:GLY:N  | 2        | 30.9          |
| (1,141) | 1:B:94:LEU:N  | 1:B:94:LEU:CA  | 1:B:94:LEU:C  | 1:B:95:GLY:N  | 2        | 30.9          |
| (1,28)  | 1:A:94:LEU:N  | 1:A:94:LEU:CA  | 1:A:94:LEU:C  | 1:A:95:GLY:N  | 9        | 30.3          |
| (1,141) | 1:B:94:LEU:N  | 1:B:94:LEU:CA  | 1:B:94:LEU:C  | 1:B:95:GLY:N  | 9        | 30.3          |
| (1,60)  | 1:A:115:SER:N | 1:A:115:SER:CA | 1:A:115:SER:C | 1:A:116:ARG:N | 4        | 30.1          |
| (1,173) | 1:B:115:SER:N | 1:B:115:SER:CA | 1:B:115:SER:C | 1:B:116:ARG:N | 4        | 30.1          |
| (1,26)  | 1:A:93:VAL:N  | 1:A:93:VAL:CA  | 1:A:93:VAL:C  | 1:A:94:LEU:N  | 7        | 29.6          |
| (1,139) | 1:B:93:VAL:N  | 1:B:93:VAL:CA  | 1:B:93:VAL:C  | 1:B:94:LEU:N  | 7        | 29.6          |
| (1,60)  | 1:A:115:SER:N | 1:A:115:SER:CA | 1:A:115:SER:C | 1:A:116:ARG:N | 2        | 29.0          |
| (1,173) | 1:B:115:SER:N | 1:B:115:SER:CA | 1:B:115:SER:C | 1:B:116:ARG:N | 2        | 29.0          |
| (1,163) | 1:B:107:ARG:N | 1:B:107:ARG:CA | 1:B:107:ARG:C | 1:B:108:GLN:N | 2        | 29.0          |
| (1,50)  | 1:A:107:ARG:N | 1:A:107:ARG:CA | 1:A:107:ARG:C | 1:A:108:GLN:N | 2        | 28.9          |
| (1,28)  | 1:A:94:LEU:N  | 1:A:94:LEU:CA  | 1:A:94:LEU:C  | 1:A:95:GLY:N  | 4        | 28.8          |
| (1,18)  | 1:A:89:LEU:N  | 1:A:89:LEU:CA  | 1:A:89:LEU:C  | 1:A:90:LYS:N  | 1        | 28.8          |
| (1,141) | 1:B:94:LEU:N  | 1:B:94:LEU:CA  | 1:B:94:LEU:C  | 1:B:95:GLY:N  | 4        | 28.8          |
| (1,131) | 1:B:89:LEU:N  | 1:B:89:LEU:CA  | 1:B:89:LEU:C  | 1:B:90:LYS:N  | 1        | 28.8          |
| (1,141) | 1:B:94:LEU:N  | 1:B:94:LEU:CA  | 1:B:94:LEU:C  | 1:B:95:GLY:N  | 7        | 28.5          |
| (1,28)  | 1:A:94:LEU:N  | 1:A:94:LEU:CA  | 1:A:94:LEU:C  | 1:A:95:GLY:N  | 7        | 28.3          |
| (1,20)  | 1:A:90:LYS:N  | 1:A:90:LYS:CA  | 1:A:90:LYS:C  | 1:A:91:VAL:N  | 4        | 28.3          |
| (1,181) | 1:B:119:HIS:N | 1:B:119:HIS:CA | 1:B:119:HIS:C | 1:B:120:ARG:N | 6        | 28.3          |
| (1,133) | 1:B:90:LYS:N  | 1:B:90:LYS:CA  | 1:B:90:LYS:C  | 1:B:91:VAL:N  | 4        | 28.3          |
| (1,68)  | 1:A:119:HIS:N | 1:A:119:HIS:CA | 1:A:119:HIS:C | 1:A:120:ARG:N | 6        | 28.2          |
| (1,62)  | 1:A:116:ARG:N | 1:A:116:ARG:CA | 1:A:116:ARG:C | 1:A:117:GLU:N | 8        | 27.8          |
| (1,175) | 1:B:116:ARG:N | 1:B:116:ARG:CA | 1:B:116:ARG:C | 1:B:117:GLU:N | 8        | 27.8          |
| (1,24)  | 1:A:92:LYS:N  | 1:A:92:LYS:CA  | 1:A:92:LYS:C  | 1:A:93:VAL:N  | 9        | 27.3          |
| (1,137) | 1:B:92:LYS:N  | 1:B:92:LYS:CA  | 1:B:92:LYS:C  | 1:B:93:VAL:N  | 9        | 27.3          |
| (1,151) | 1:B:101:HIS:N | 1:B:101:HIS:CA | 1:B:101:HIS:C | 1:B:102:GLY:N | 9        | 27.1          |
| (1,38)  | 1:A:101:HIS:N | 1:A:101:HIS:CA | 1:A:101:HIS:C | 1:A:102:GLY:N | 9        | 27.0          |
| (1,147) | 1:B:99:GLU:N  | 1:B:99:GLU:CA  | 1:B:99:GLU:C  | 1:B:100:VAL:N | 5        | 26.3          |
| (1,34)  | 1:A:99:GLU:N  | 1:A:99:GLU:CA  | 1:A:99:GLU:C  | 1:A:100:VAL:N | 5        | 26.2          |
| (1,139) | 1:B:93:VAL:N  | 1:B:93:VAL:CA  | 1:B:93:VAL:C  | 1:B:94:LEU:N  | 6        | 26.2          |
| (1,26)  | 1:A:93:VAL:N  | 1:A:93:VAL:CA  | 1:A:93:VAL:C  | 1:A:94:LEU:N  | 6        | 26.1          |
| (1,139) | 1:B:93:VAL:N  | 1:B:93:VAL:CA  | 1:B:93:VAL:C  | 1:B:94:LEU:N  | 9        | 25.9          |
| (1,26)  | 1:A:93:VAL:N  | 1:A:93:VAL:CA  | 1:A:93:VAL:C  | 1:A:94:LEU:N  | 9        | 25.8          |
| (1,34)  | 1:A:99:GLU:N  | 1:A:99:GLU:CA  | 1:A:99:GLU:C  | 1:A:100:VAL:N | 4        | 25.7          |
| (1,147) | 1:B:99:GLU:N  | 1:B:99:GLU:CA  | 1:B:99:GLU:C  | 1:B:100:VAL:N | 4        | 25.6          |
| (1,26)  | 1:A:93:VAL:N  | 1:A:93:VAL:CA  | 1:A:93:VAL:C  | 1:A:94:LEU:N  | 4        | 25.3          |
| (1,24)  | 1:A:92:LYS:N  | 1:A:92:LYS:CA  | 1:A:92:LYS:C  | 1:A:93:VAL:N  | 7        | 25.3          |
| (1,139) | 1:B:93:VAL:N  | 1:B:93:VAL:CA  | 1:B:93:VAL:C  | 1:B:94:LEU:N  | 4        | 25.3          |
| (1,137) | 1:B:92:LYS:N  | 1:B:92:LYS:CA  | 1:B:92:LYS:C  | 1:B:93:VAL:N  | 7        | 25.3          |
| (1,28)  | 1:A:94:LEU:N  | 1:A:94:LEU:CA  | 1:A:94:LEU:C  | 1:A:95:GLY:N  | 1        | 25.2          |
| (1,60)  | 1:A:115:SER:N | 1:A:115:SER:CA | 1:A:115:SER:C | 1:A:116:ARG:N | 8        | 25.1          |
| (1,121) | 1:B:78:ASN:N  | 1:B:78:ASN:CA  | 1:B:78:ASN:C  | 1:B:79:LEU:N  | 4        | 25.1          |
| (1,8)   | 1:A:78:ASN:N  | 1:A:78:ASN:CA  | 1:A:78:ASN:C  | 1:A:79:LEU:N  | 4        | 25.0          |
| (1,173) | 1:B:115:SER:N | 1:B:115:SER:CA | 1:B:115:SER:C | 1:B:116:ARG:N | 8        | 25.0          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,141) | 1:B:94:LEU:N  | 1:B:94:LEU:CA  | 1:B:94:LEU:C   | 1:B:95:GLY:N  | 1        | 25.0          |
| (1,113) | 1:A:146:ASP:N | 1:A:146:ASP:CA | 1:A:146:ASP:C  | 1:A:147:GLY:N | 6        | 25.0          |
| (1,226) | 1:B:146:ASP:N | 1:B:146:ASP:CA | 1:B:146:ASP:C  | 1:B:147:GLY:N | 6        | 24.9          |
| (1,36)  | 1:A:100:VAL:N | 1:A:100:VAL:CA | 1:A:100:VAL:C  | 1:A:101:HIS:N | 5        | 24.7          |
| (1,149) | 1:B:100:VAL:N | 1:B:100:VAL:CA | 1:B:100:VAL:C  | 1:B:101:HIS:N | 5        | 24.6          |
| (1,164) | 1:B:107:ARG:C | 1:B:108:GLN:N  | 1:B:108:GLN:CA | 1:B:108:GLN:C | 6        | 24.0          |
| (1,33)  | 1:A:98:ILE:C  | 1:A:99:GLU:N   | 1:A:99:GLU:CA  | 1:A:99:GLU:C  | 7        | 23.9          |
| (1,146) | 1:B:98:ILE:C  | 1:B:99:GLU:N   | 1:B:99:GLU:CA  | 1:B:99:GLU:C  | 7        | 23.9          |
| (1,69)  | 1:A:119:HIS:C | 1:A:120:ARG:N  | 1:A:120:ARG:CA | 1:A:120:ARG:C | 9        | 23.8          |
| (1,51)  | 1:A:107:ARG:C | 1:A:108:GLN:N  | 1:A:108:GLN:CA | 1:A:108:GLN:C | 6        | 23.8          |
| (1,26)  | 1:A:93:VAL:N  | 1:A:93:VAL:CA  | 1:A:93:VAL:C   | 1:A:94:LEU:N  | 5        | 23.8          |
| (1,20)  | 1:A:90:LYS:N  | 1:A:90:LYS:CA  | 1:A:90:LYS:C   | 1:A:91:VAL:N  | 3        | 23.8          |
| (1,182) | 1:B:119:HIS:C | 1:B:120:ARG:N  | 1:B:120:ARG:CA | 1:B:120:ARG:C | 9        | 23.8          |
| (1,139) | 1:B:93:VAL:N  | 1:B:93:VAL:CA  | 1:B:93:VAL:C   | 1:B:94:LEU:N  | 5        | 23.7          |
| (1,133) | 1:B:90:LYS:N  | 1:B:90:LYS:CA  | 1:B:90:LYS:C   | 1:B:91:VAL:N  | 3        | 23.7          |
| (1,9)   | 1:A:78:ASN:C  | 1:A:79:LEU:N   | 1:A:79:LEU:CA  | 1:A:79:LEU:C  | 4        | 23.5          |
| (1,122) | 1:B:78:ASN:C  | 1:B:79:LEU:N   | 1:B:79:LEU:CA  | 1:B:79:LEU:C  | 4        | 23.5          |
| (1,50)  | 1:A:107:ARG:N | 1:A:107:ARG:CA | 1:A:107:ARG:C  | 1:A:108:GLN:N | 1        | 23.4          |
| (1,33)  | 1:A:98:ILE:C  | 1:A:99:GLU:N   | 1:A:99:GLU:CA  | 1:A:99:GLU:C  | 4        | 23.4          |
| (1,146) | 1:B:98:ILE:C  | 1:B:99:GLU:N   | 1:B:99:GLU:CA  | 1:B:99:GLU:C  | 4        | 23.4          |
| (1,39)  | 1:A:101:HIS:C | 1:A:102:GLY:N  | 1:A:102:GLY:CA | 1:A:102:GLY:C | 6        | 23.3          |
| (1,163) | 1:B:107:ARG:N | 1:B:107:ARG:CA | 1:B:107:ARG:C  | 1:B:108:GLN:N | 1        | 23.3          |
| (1,152) | 1:B:101:HIS:C | 1:B:102:GLY:N  | 1:B:102:GLY:CA | 1:B:102:GLY:C | 6        | 23.2          |
| (1,218) | 1:B:142:VAL:N | 1:B:142:VAL:CA | 1:B:142:VAL:C  | 1:B:143:LEU:N | 4        | 22.8          |
| (1,105) | 1:A:142:VAL:N | 1:A:142:VAL:CA | 1:A:142:VAL:C  | 1:A:143:LEU:N | 4        | 22.7          |
| (1,33)  | 1:A:98:ILE:C  | 1:A:99:GLU:N   | 1:A:99:GLU:CA  | 1:A:99:GLU:C  | 5        | 22.6          |
| (1,146) | 1:B:98:ILE:C  | 1:B:99:GLU:N   | 1:B:99:GLU:CA  | 1:B:99:GLU:C  | 5        | 22.5          |
| (1,24)  | 1:A:92:LYS:N  | 1:A:92:LYS:CA  | 1:A:92:LYS:C   | 1:A:93:VAL:N  | 5        | 22.4          |
| (1,39)  | 1:A:101:HIS:C | 1:A:102:GLY:N  | 1:A:102:GLY:CA | 1:A:102:GLY:C | 5        | 22.3          |
| (1,163) | 1:B:107:ARG:N | 1:B:107:ARG:CA | 1:B:107:ARG:C  | 1:B:108:GLN:N | 6        | 22.3          |
| (1,152) | 1:B:101:HIS:C | 1:B:102:GLY:N  | 1:B:102:GLY:CA | 1:B:102:GLY:C | 5        | 22.3          |
| (1,137) | 1:B:92:LYS:N  | 1:B:92:LYS:CA  | 1:B:92:LYS:C   | 1:B:93:VAL:N  | 5        | 22.3          |
| (1,50)  | 1:A:107:ARG:N | 1:A:107:ARG:CA | 1:A:107:ARG:C  | 1:A:108:GLN:N | 6        | 22.2          |
| (1,24)  | 1:A:92:LYS:N  | 1:A:92:LYS:CA  | 1:A:92:LYS:C   | 1:A:93:VAL:N  | 6        | 22.2          |
| (1,137) | 1:B:92:LYS:N  | 1:B:92:LYS:CA  | 1:B:92:LYS:C   | 1:B:93:VAL:N  | 6        | 22.2          |
| (1,63)  | 1:A:116:ARG:C | 1:A:117:GLU:N  | 1:A:117:GLU:CA | 1:A:117:GLU:C | 7        | 22.1          |
| (1,50)  | 1:A:107:ARG:N | 1:A:107:ARG:CA | 1:A:107:ARG:C  | 1:A:108:GLN:N | 8        | 22.1          |
| (1,176) | 1:B:116:ARG:C | 1:B:117:GLU:N  | 1:B:117:GLU:CA | 1:B:117:GLU:C | 7        | 22.1          |
| (1,163) | 1:B:107:ARG:N | 1:B:107:ARG:CA | 1:B:107:ARG:C  | 1:B:108:GLN:N | 8        | 22.0          |
| (1,32)  | 1:A:98:ILE:N  | 1:A:98:ILE:CA  | 1:A:98:ILE:C   | 1:A:99:GLU:N  | 6        | 21.8          |
| (1,63)  | 1:A:116:ARG:C | 1:A:117:GLU:N  | 1:A:117:GLU:CA | 1:A:117:GLU:C | 8        | 21.6          |
| (1,18)  | 1:A:89:LEU:N  | 1:A:89:LEU:CA  | 1:A:89:LEU:C   | 1:A:90:LYS:N  | 3        | 21.6          |
| (1,175) | 1:B:116:ARG:N | 1:B:116:ARG:CA | 1:B:116:ARG:C  | 1:B:117:GLU:N | 2        | 21.6          |
| (1,62)  | 1:A:116:ARG:N | 1:A:116:ARG:CA | 1:A:116:ARG:C  | 1:A:117:GLU:N | 2        | 21.5          |
| (1,176) | 1:B:116:ARG:C | 1:B:117:GLU:N  | 1:B:117:GLU:CA | 1:B:117:GLU:C | 8        | 21.5          |
| (1,145) | 1:B:98:ILE:N  | 1:B:98:ILE:CA  | 1:B:98:ILE:C   | 1:B:99:GLU:N  | 6        | 21.5          |
| (1,131) | 1:B:89:LEU:N  | 1:B:89:LEU:CA  | 1:B:89:LEU:C   | 1:B:90:LYS:N  | 3        | 21.5          |
| (1,226) | 1:B:146:ASP:N | 1:B:146:ASP:CA | 1:B:146:ASP:C  | 1:B:147:GLY:N | 1        | 21.4          |
| (1,53)  | 1:A:110:GLU:C | 1:A:111:HIS:N  | 1:A:111:HIS:CA | 1:A:111:HIS:C | 1        | 21.2          |
| (1,166) | 1:B:110:GLU:C | 1:B:111:HIS:N  | 1:B:111:HIS:CA | 1:B:111:HIS:C | 1        | 21.2          |
| (1,113) | 1:A:146:ASP:N | 1:A:146:ASP:CA | 1:A:146:ASP:C  | 1:A:147:GLY:N | 1        | 21.2          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,34)  | 1:A:99:GLU:N  | 1:A:99:GLU:CA  | 1:A:99:GLU:C   | 1:A:100:VAL:N | 7        | 21.1          |
| (1,28)  | 1:A:94:LEU:N  | 1:A:94:LEU:CA  | 1:A:94:LEU:C   | 1:A:95:GLY:N  | 8        | 21.1          |
| (1,147) | 1:B:99:GLU:N  | 1:B:99:GLU:CA  | 1:B:99:GLU:C   | 1:B:100:VAL:N | 7        | 21.1          |
| (1,141) | 1:B:94:LEU:N  | 1:B:94:LEU:CA  | 1:B:94:LEU:C   | 1:B:95:GLY:N  | 8        | 21.1          |
| (1,33)  | 1:A:98:ILE:C  | 1:A:99:GLU:N   | 1:A:99:GLU:CA  | 1:A:99:GLU:C  | 3        | 20.9          |
| (1,146) | 1:B:98:ILE:C  | 1:B:99:GLU:N   | 1:B:99:GLU:CA  | 1:B:99:GLU:C  | 3        | 20.8          |
| (1,85)  | 1:A:130:PRO:N | 1:A:130:PRO:CA | 1:A:130:PRO:C  | 1:A:131:LEU:N | 2        | 20.5          |
| (1,36)  | 1:A:100:VAL:N | 1:A:100:VAL:CA | 1:A:100:VAL:C  | 1:A:101:HIS:N | 8        | 20.4          |
| (1,198) | 1:B:130:PRO:N | 1:B:130:PRO:CA | 1:B:130:PRO:C  | 1:B:131:LEU:N | 2        | 20.4          |
| (1,164) | 1:B:107:ARG:C | 1:B:108:GLN:N  | 1:B:108:GLN:CA | 1:B:108:GLN:C | 2        | 20.4          |
| (1,149) | 1:B:100:VAL:N | 1:B:100:VAL:CA | 1:B:100:VAL:C  | 1:B:101:HIS:N | 8        | 20.4          |
| (1,51)  | 1:A:107:ARG:C | 1:A:108:GLN:N  | 1:A:108:GLN:CA | 1:A:108:GLN:C | 2        | 20.3          |
| (1,17)  | 1:A:88:GLU:C  | 1:A:89:LEU:N   | 1:A:89:LEU:CA  | 1:A:89:LEU:C  | 7        | 20.3          |
| (1,150) | 1:B:100:VAL:C | 1:B:101:HIS:N  | 1:B:101:HIS:CA | 1:B:101:HIS:C | 9        | 20.1          |
| (1,130) | 1:B:88:GLU:C  | 1:B:89:LEU:N   | 1:B:89:LEU:CA  | 1:B:89:LEU:C  | 7        | 20.1          |
| (1,37)  | 1:A:100:VAL:C | 1:A:101:HIS:N  | 1:A:101:HIS:CA | 1:A:101:HIS:C | 9        | 19.8          |
| (1,92)  | 1:A:134:THR:C | 1:A:135:SER:N  | 1:A:135:SER:CA | 1:A:135:SER:C | 2        | 19.6          |
| (1,164) | 1:B:107:ARG:C | 1:B:108:GLN:N  | 1:B:108:GLN:CA | 1:B:108:GLN:C | 4        | 19.6          |
| (1,56)  | 1:A:113:PHE:N | 1:A:113:PHE:CA | 1:A:113:PHE:C  | 1:A:114:ILE:N | 3        | 19.5          |
| (1,205) | 1:B:134:THR:C | 1:B:135:SER:N  | 1:B:135:SER:CA | 1:B:135:SER:C | 2        | 19.5          |
| (1,169) | 1:B:113:PHE:N | 1:B:113:PHE:CA | 1:B:113:PHE:C  | 1:B:114:ILE:N | 3        | 19.5          |
| (1,51)  | 1:A:107:ARG:C | 1:A:108:GLN:N  | 1:A:108:GLN:CA | 1:A:108:GLN:C | 4        | 19.4          |
| (1,134) | 1:B:90:LYS:C  | 1:B:91:VAL:N   | 1:B:91:VAL:CA  | 1:B:91:VAL:C  | 4        | 19.3          |
| (1,26)  | 1:A:93:VAL:N  | 1:A:93:VAL:CA  | 1:A:93:VAL:C   | 1:A:94:LEU:N  | 3        | 19.1          |
| (1,21)  | 1:A:90:LYS:C  | 1:A:91:VAL:N   | 1:A:91:VAL:CA  | 1:A:91:VAL:C  | 4        | 19.1          |
| (1,139) | 1:B:93:VAL:N  | 1:B:93:VAL:CA  | 1:B:93:VAL:C   | 1:B:94:LEU:N  | 3        | 19.1          |
| (1,6)   | 1:A:77:VAL:N  | 1:A:77:VAL:CA  | 1:A:77:VAL:C   | 1:A:78:ASN:N  | 5        | 19.0          |
| (1,119) | 1:B:77:VAL:N  | 1:B:77:VAL:CA  | 1:B:77:VAL:C   | 1:B:78:ASN:N  | 5        | 19.0          |
| (1,41)  | 1:A:102:GLY:C | 1:A:103:LYS:N  | 1:A:103:LYS:CA | 1:A:103:LYS:C | 7        | 18.9          |
| (1,154) | 1:B:102:GLY:C | 1:B:103:LYS:N  | 1:B:103:LYS:CA | 1:B:103:LYS:C | 7        | 18.9          |
| (1,20)  | 1:A:90:LYS:N  | 1:A:90:LYS:CA  | 1:A:90:LYS:C   | 1:A:91:VAL:N  | 1        | 18.6          |
| (1,133) | 1:B:90:LYS:N  | 1:B:90:LYS:CA  | 1:B:90:LYS:C   | 1:B:91:VAL:N  | 1        | 18.6          |
| (1,57)  | 1:A:113:PHE:C | 1:A:114:ILE:N  | 1:A:114:ILE:CA | 1:A:114:ILE:C | 3        | 18.5          |
| (1,170) | 1:B:113:PHE:C | 1:B:114:ILE:N  | 1:B:114:ILE:CA | 1:B:114:ILE:C | 3        | 18.5          |
| (1,92)  | 1:A:134:THR:C | 1:A:135:SER:N  | 1:A:135:SER:CA | 1:A:135:SER:C | 3        | 18.2          |
| (1,21)  | 1:A:90:LYS:C  | 1:A:91:VAL:N   | 1:A:91:VAL:CA  | 1:A:91:VAL:C  | 1        | 18.2          |
| (1,205) | 1:B:134:THR:C | 1:B:135:SER:N  | 1:B:135:SER:CA | 1:B:135:SER:C | 3        | 18.2          |
| (1,134) | 1:B:90:LYS:C  | 1:B:91:VAL:N   | 1:B:91:VAL:CA  | 1:B:91:VAL:C  | 1        | 18.1          |
| (1,46)  | 1:A:105:GLU:N | 1:A:105:GLU:CA | 1:A:105:GLU:C  | 1:A:106:GLU:N | 4        | 18.0          |
| (1,35)  | 1:A:99:GLU:C  | 1:A:100:VAL:N  | 1:A:100:VAL:CA | 1:A:100:VAL:C | 5        | 17.9          |
| (1,33)  | 1:A:98:ILE:C  | 1:A:99:GLU:N   | 1:A:99:GLU:CA  | 1:A:99:GLU:C  | 6        | 17.9          |
| (1,159) | 1:B:105:GLU:N | 1:B:105:GLU:CA | 1:B:105:GLU:C  | 1:B:106:GLU:N | 4        | 17.9          |
| (1,32)  | 1:A:98:ILE:N  | 1:A:98:ILE:CA  | 1:A:98:ILE:C   | 1:A:99:GLU:N  | 3        | 17.8          |
| (1,149) | 1:B:100:VAL:N | 1:B:100:VAL:CA | 1:B:100:VAL:C  | 1:B:101:HIS:N | 9        | 17.8          |
| (1,148) | 1:B:99:GLU:C  | 1:B:100:VAL:N  | 1:B:100:VAL:CA | 1:B:100:VAL:C | 5        | 17.8          |
| (1,146) | 1:B:98:ILE:C  | 1:B:99:GLU:N   | 1:B:99:GLU:CA  | 1:B:99:GLU:C  | 6        | 17.8          |
| (1,145) | 1:B:98:ILE:N  | 1:B:98:ILE:CA  | 1:B:98:ILE:C   | 1:B:99:GLU:N  | 3        | 17.7          |
| (1,137) | 1:B:92:LYS:N  | 1:B:92:LYS:CA  | 1:B:92:LYS:C   | 1:B:93:VAL:N  | 3        | 17.7          |
| (1,24)  | 1:A:92:LYS:N  | 1:A:92:LYS:CA  | 1:A:92:LYS:C   | 1:A:93:VAL:N  | 3        | 17.6          |
| (1,36)  | 1:A:100:VAL:N | 1:A:100:VAL:CA | 1:A:100:VAL:C  | 1:A:101:HIS:N | 9        | 17.5          |
| (1,67)  | 1:A:118:PHE:C | 1:A:119:HIS:N  | 1:A:119:HIS:CA | 1:A:119:HIS:C | 8        | 17.4          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,53)  | 1:A:110:GLU:C | 1:A:111:HIS:N  | 1:A:111:HIS:CA | 1:A:111:HIS:C | 5        | 17.4          |
| (1,180) | 1:B:118:PHE:C | 1:B:119:HIS:N  | 1:B:119:HIS:CA | 1:B:119:HIS:C | 8        | 17.4          |
| (1,166) | 1:B:110:GLU:C | 1:B:111:HIS:N  | 1:B:111:HIS:CA | 1:B:111:HIS:C | 5        | 17.4          |
| (1,69)  | 1:A:119:HIS:C | 1:A:120:ARG:N  | 1:A:120:ARG:CA | 1:A:120:ARG:C | 6        | 17.3          |
| (1,182) | 1:B:119:HIS:C | 1:B:120:ARG:N  | 1:B:120:ARG:CA | 1:B:120:ARG:C | 6        | 17.3          |
| (1,26)  | 1:A:93:VAL:N  | 1:A:93:VAL:CA  | 1:A:93:VAL:C   | 1:A:94:LEU:N  | 1        | 17.2          |
| (1,149) | 1:B:100:VAL:N | 1:B:100:VAL:CA | 1:B:100:VAL:C  | 1:B:101:HIS:N | 6        | 17.2          |
| (1,139) | 1:B:93:VAL:N  | 1:B:93:VAL:CA  | 1:B:93:VAL:C   | 1:B:94:LEU:N  | 1        | 17.2          |
| (1,36)  | 1:A:100:VAL:N | 1:A:100:VAL:CA | 1:A:100:VAL:C  | 1:A:101:HIS:N | 6        | 17.1          |
| (1,68)  | 1:A:119:HIS:N | 1:A:119:HIS:CA | 1:A:119:HIS:C  | 1:A:120:ARG:N | 9        | 17.0          |
| (1,226) | 1:B:146:ASP:N | 1:B:146:ASP:CA | 1:B:146:ASP:C  | 1:B:147:GLY:N | 9        | 17.0          |
| (1,181) | 1:B:119:HIS:N | 1:B:119:HIS:CA | 1:B:119:HIS:C  | 1:B:120:ARG:N | 4        | 17.0          |
| (1,181) | 1:B:119:HIS:N | 1:B:119:HIS:CA | 1:B:119:HIS:C  | 1:B:120:ARG:N | 9        | 17.0          |
| (1,113) | 1:A:146:ASP:N | 1:A:146:ASP:CA | 1:A:146:ASP:C  | 1:A:147:GLY:N | 9        | 17.0          |
| (1,68)  | 1:A:119:HIS:N | 1:A:119:HIS:CA | 1:A:119:HIS:C  | 1:A:120:ARG:N | 4        | 16.9          |
| (1,150) | 1:B:100:VAL:C | 1:B:101:HIS:N  | 1:B:101:HIS:CA | 1:B:101:HIS:C | 4        | 16.9          |
| (1,37)  | 1:A:100:VAL:C | 1:A:101:HIS:N  | 1:A:101:HIS:CA | 1:A:101:HIS:C | 4        | 16.7          |
| (1,34)  | 1:A:99:GLU:N  | 1:A:99:GLU:CA  | 1:A:99:GLU:C   | 1:A:100:VAL:N | 1        | 16.7          |
| (1,28)  | 1:A:94:LEU:N  | 1:A:94:LEU:CA  | 1:A:94:LEU:C   | 1:A:95:GLY:N  | 6        | 16.7          |
| (1,147) | 1:B:99:GLU:N  | 1:B:99:GLU:CA  | 1:B:99:GLU:C   | 1:B:100:VAL:N | 1        | 16.7          |
| (1,141) | 1:B:94:LEU:N  | 1:B:94:LEU:CA  | 1:B:94:LEU:C   | 1:B:95:GLY:N  | 6        | 16.7          |
| (1,48)  | 1:A:106:GLU:N | 1:A:106:GLU:CA | 1:A:106:GLU:C  | 1:A:107:ARG:N | 2        | 16.6          |
| (1,91)  | 1:A:134:THR:N | 1:A:134:THR:CA | 1:A:134:THR:C  | 1:A:135:SER:N | 4        | 16.5          |
| (1,161) | 1:B:106:GLU:N | 1:B:106:GLU:CA | 1:B:106:GLU:C  | 1:B:107:ARG:N | 2        | 16.5          |
| (1,154) | 1:B:102:GLY:C | 1:B:103:LYS:N  | 1:B:103:LYS:CA | 1:B:103:LYS:C | 8        | 16.5          |
| (1,41)  | 1:A:102:GLY:C | 1:A:103:LYS:N  | 1:A:103:LYS:CA | 1:A:103:LYS:C | 8        | 16.4          |
| (1,204) | 1:B:134:THR:N | 1:B:134:THR:CA | 1:B:134:THR:C  | 1:B:135:SER:N | 4        | 16.4          |
| (1,173) | 1:B:115:SER:N | 1:B:115:SER:CA | 1:B:115:SER:C  | 1:B:116:ARG:N | 7        | 16.4          |
| (1,67)  | 1:A:118:PHE:C | 1:A:119:HIS:N  | 1:A:119:HIS:CA | 1:A:119:HIS:C | 7        | 16.3          |
| (1,60)  | 1:A:115:SER:N | 1:A:115:SER:CA | 1:A:115:SER:C  | 1:A:116:ARG:N | 7        | 16.3          |
| (1,180) | 1:B:118:PHE:C | 1:B:119:HIS:N  | 1:B:119:HIS:CA | 1:B:119:HIS:C | 7        | 16.2          |
| (1,69)  | 1:A:119:HIS:C | 1:A:120:ARG:N  | 1:A:120:ARG:CA | 1:A:120:ARG:C | 3        | 16.0          |
| (1,69)  | 1:A:119:HIS:C | 1:A:120:ARG:N  | 1:A:120:ARG:CA | 1:A:120:ARG:C | 5        | 16.0          |
| (1,182) | 1:B:119:HIS:C | 1:B:120:ARG:N  | 1:B:120:ARG:CA | 1:B:120:ARG:C | 3        | 16.0          |
| (1,182) | 1:B:119:HIS:C | 1:B:120:ARG:N  | 1:B:120:ARG:CA | 1:B:120:ARG:C | 5        | 16.0          |
| (1,29)  | 1:A:96:ASP:C  | 1:A:97:VAL:N   | 1:A:97:VAL:CA  | 1:A:97:VAL:C  | 6        | 15.9          |
| (1,142) | 1:B:96:ASP:C  | 1:B:97:VAL:N   | 1:B:97:VAL:CA  | 1:B:97:VAL:C  | 6        | 15.9          |
| (1,69)  | 1:A:119:HIS:C | 1:A:120:ARG:N  | 1:A:120:ARG:CA | 1:A:120:ARG:C | 2        | 15.5          |
| (1,182) | 1:B:119:HIS:C | 1:B:120:ARG:N  | 1:B:120:ARG:CA | 1:B:120:ARG:C | 2        | 15.5          |
| (1,58)  | 1:A:114:ILE:N | 1:A:114:ILE:CA | 1:A:114:ILE:C  | 1:A:115:SER:N | 5        | 15.4          |
| (1,183) | 1:B:120:ARG:N | 1:B:120:ARG:CA | 1:B:120:ARG:C  | 1:B:121:LYS:N | 1        | 15.4          |
| (1,171) | 1:B:114:ILE:N | 1:B:114:ILE:CA | 1:B:114:ILE:C  | 1:B:115:SER:N | 5        | 15.4          |
| (1,70)  | 1:A:120:ARG:N | 1:A:120:ARG:CA | 1:A:120:ARG:C  | 1:A:121:LYS:N | 1        | 15.3          |
| (1,69)  | 1:A:119:HIS:C | 1:A:120:ARG:N  | 1:A:120:ARG:CA | 1:A:120:ARG:C | 1        | 15.3          |
| (1,53)  | 1:A:110:GLU:C | 1:A:111:HIS:N  | 1:A:111:HIS:CA | 1:A:111:HIS:C | 7        | 15.3          |
| (1,182) | 1:B:119:HIS:C | 1:B:120:ARG:N  | 1:B:120:ARG:CA | 1:B:120:ARG:C | 1        | 15.3          |
| (1,166) | 1:B:110:GLU:C | 1:B:111:HIS:N  | 1:B:111:HIS:CA | 1:B:111:HIS:C | 7        | 15.3          |
| (1,66)  | 1:A:118:PHE:N | 1:A:118:PHE:CA | 1:A:118:PHE:C  | 1:A:119:HIS:N | 3        | 15.2          |
| (1,179) | 1:B:118:PHE:N | 1:B:118:PHE:CA | 1:B:118:PHE:C  | 1:B:119:HIS:N | 3        | 15.1          |
| (1,111) | 1:A:145:VAL:N | 1:A:145:VAL:CA | 1:A:145:VAL:C  | 1:A:146:ASP:N | 6        | 14.8          |
| (1,73)  | 1:A:121:LYS:C | 1:A:122:TYR:N  | 1:A:122:TYR:CA | 1:A:122:TYR:C | 9        | 14.7          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,224) | 1:B:145:VAL:N | 1:B:145:VAL:CA | 1:B:145:VAL:C  | 1:B:146:ASP:N | 6        | 14.7          |
| (1,186) | 1:B:121:LYS:C | 1:B:122:TYR:N  | 1:B:122:TYR:CA | 1:B:122:TYR:C | 9        | 14.6          |
| (1,147) | 1:B:99:GLU:N  | 1:B:99:GLU:CA  | 1:B:99:GLU:C   | 1:B:100:VAL:N | 2        | 14.5          |
| (1,222) | 1:B:144:THR:N | 1:B:144:THR:CA | 1:B:144:THR:C  | 1:B:145:VAL:N | 2        | 14.4          |
| (1,66)  | 1:A:118:PHE:N | 1:A:118:PHE:CA | 1:A:118:PHE:C  | 1:A:119:HIS:N | 9        | 14.3          |
| (1,37)  | 1:A:100:VAL:C | 1:A:101:HIS:N  | 1:A:101:HIS:CA | 1:A:101:HIS:C | 2        | 14.3          |
| (1,34)  | 1:A:99:GLU:N  | 1:A:99:GLU:CA  | 1:A:99:GLU:C   | 1:A:100:VAL:N | 2        | 14.3          |
| (1,179) | 1:B:118:PHE:N | 1:B:118:PHE:CA | 1:B:118:PHE:C  | 1:B:119:HIS:N | 9        | 14.3          |
| (1,109) | 1:A:144:THR:N | 1:A:144:THR:CA | 1:A:144:THR:C  | 1:A:145:VAL:N | 2        | 14.3          |
| (1,60)  | 1:A:115:SER:N | 1:A:115:SER:CA | 1:A:115:SER:C  | 1:A:116:ARG:N | 5        | 14.2          |
| (1,173) | 1:B:115:SER:N | 1:B:115:SER:CA | 1:B:115:SER:C  | 1:B:116:ARG:N | 5        | 14.2          |
| (1,150) | 1:B:100:VAL:C | 1:B:101:HIS:N  | 1:B:101:HIS:CA | 1:B:101:HIS:C | 2        | 14.2          |
| (1,39)  | 1:A:101:HIS:C | 1:A:102:GLY:N  | 1:A:102:GLY:CA | 1:A:102:GLY:C | 7        | 14.0          |
| (1,152) | 1:B:101:HIS:C | 1:B:102:GLY:N  | 1:B:102:GLY:CA | 1:B:102:GLY:C | 7        | 14.0          |
| (1,32)  | 1:A:98:ILE:N  | 1:A:98:ILE:CA  | 1:A:98:ILE:C   | 1:A:99:GLU:N  | 7        | 13.5          |
| (1,145) | 1:B:98:ILE:N  | 1:B:98:ILE:CA  | 1:B:98:ILE:C   | 1:B:99:GLU:N  | 7        | 13.5          |
| (1,105) | 1:A:142:VAL:N | 1:A:142:VAL:CA | 1:A:142:VAL:C  | 1:A:143:LEU:N | 5        | 13.5          |
| (1,218) | 1:B:142:VAL:N | 1:B:142:VAL:CA | 1:B:142:VAL:C  | 1:B:143:LEU:N | 5        | 13.4          |
| (1,39)  | 1:A:101:HIS:C | 1:A:102:GLY:N  | 1:A:102:GLY:CA | 1:A:102:GLY:C | 8        | 13.3          |
| (1,152) | 1:B:101:HIS:C | 1:B:102:GLY:N  | 1:B:102:GLY:CA | 1:B:102:GLY:C | 8        | 13.3          |
| (1,134) | 1:B:90:LYS:C  | 1:B:91:VAL:N   | 1:B:91:VAL:CA  | 1:B:91:VAL:C  | 7        | 13.1          |
| (1,21)  | 1:A:90:LYS:C  | 1:A:91:VAL:N   | 1:A:91:VAL:CA  | 1:A:91:VAL:C  | 7        | 13.0          |
| (1,18)  | 1:A:89:LEU:N  | 1:A:89:LEU:CA  | 1:A:89:LEU:C   | 1:A:90:LYS:N  | 8        | 12.8          |
| (1,131) | 1:B:89:LEU:N  | 1:B:89:LEU:CA  | 1:B:89:LEU:C   | 1:B:90:LYS:N  | 8        | 12.7          |
| (1,4)   | 1:A:76:SER:N  | 1:A:76:SER:CA  | 1:A:76:SER:C   | 1:A:77:VAL:N  | 9        | 12.5          |
| (1,145) | 1:B:98:ILE:N  | 1:B:98:ILE:CA  | 1:B:98:ILE:C   | 1:B:99:GLU:N  | 8        | 12.5          |
| (1,117) | 1:B:76:SER:N  | 1:B:76:SER:CA  | 1:B:76:SER:C   | 1:B:77:VAL:N  | 9        | 12.5          |
| (1,32)  | 1:A:98:ILE:N  | 1:A:98:ILE:CA  | 1:A:98:ILE:C   | 1:A:99:GLU:N  | 8        | 12.4          |
| (1,41)  | 1:A:102:GLY:C | 1:A:103:LYS:N  | 1:A:103:LYS:CA | 1:A:103:LYS:C | 2        | 12.3          |
| (1,33)  | 1:A:98:ILE:C  | 1:A:99:GLU:N   | 1:A:99:GLU:CA  | 1:A:99:GLU:C  | 2        | 12.3          |
| (1,146) | 1:B:98:ILE:C  | 1:B:99:GLU:N   | 1:B:99:GLU:CA  | 1:B:99:GLU:C  | 2        | 12.3          |
| (1,18)  | 1:A:89:LEU:N  | 1:A:89:LEU:CA  | 1:A:89:LEU:C   | 1:A:90:LYS:N  | 6        | 12.2          |
| (1,154) | 1:B:102:GLY:C | 1:B:103:LYS:N  | 1:B:103:LYS:CA | 1:B:103:LYS:C | 2        | 12.2          |
| (1,147) | 1:B:99:GLU:N  | 1:B:99:GLU:CA  | 1:B:99:GLU:C   | 1:B:100:VAL:N | 6        | 12.2          |
| (1,131) | 1:B:89:LEU:N  | 1:B:89:LEU:CA  | 1:B:89:LEU:C   | 1:B:90:LYS:N  | 6        | 12.2          |
| (1,34)  | 1:A:99:GLU:N  | 1:A:99:GLU:CA  | 1:A:99:GLU:C   | 1:A:100:VAL:N | 6        | 12.0          |
| (1,32)  | 1:A:98:ILE:N  | 1:A:98:ILE:CA  | 1:A:98:ILE:C   | 1:A:99:GLU:N  | 1        | 11.9          |
| (1,179) | 1:B:118:PHE:N | 1:B:118:PHE:CA | 1:B:118:PHE:C  | 1:B:119:HIS:N | 4        | 11.9          |
| (1,66)  | 1:A:118:PHE:N | 1:A:118:PHE:CA | 1:A:118:PHE:C  | 1:A:119:HIS:N | 4        | 11.8          |
| (1,176) | 1:B:116:ARG:C | 1:B:117:GLU:N  | 1:B:117:GLU:CA | 1:B:117:GLU:C | 1        | 11.8          |
| (1,145) | 1:B:98:ILE:N  | 1:B:98:ILE:CA  | 1:B:98:ILE:C   | 1:B:99:GLU:N  | 1        | 11.8          |
| (1,133) | 1:B:90:LYS:N  | 1:B:90:LYS:CA  | 1:B:90:LYS:C   | 1:B:91:VAL:N  | 8        | 11.8          |
| (1,20)  | 1:A:90:LYS:N  | 1:A:90:LYS:CA  | 1:A:90:LYS:C   | 1:A:91:VAL:N  | 8        | 11.7          |
| (1,63)  | 1:A:116:ARG:C | 1:A:117:GLU:N  | 1:A:117:GLU:CA | 1:A:117:GLU:C | 1        | 11.6          |
| (1,111) | 1:A:145:VAL:N | 1:A:145:VAL:CA | 1:A:145:VAL:C  | 1:A:146:ASP:N | 5        | 11.5          |
| (1,224) | 1:B:145:VAL:N | 1:B:145:VAL:CA | 1:B:145:VAL:C  | 1:B:146:ASP:N | 5        | 11.4          |
| (1,37)  | 1:A:100:VAL:C | 1:A:101:HIS:N  | 1:A:101:HIS:CA | 1:A:101:HIS:C | 5        | 10.9          |
| (1,37)  | 1:A:100:VAL:C | 1:A:101:HIS:N  | 1:A:101:HIS:CA | 1:A:101:HIS:C | 7        | 10.9          |
| (1,150) | 1:B:100:VAL:C | 1:B:101:HIS:N  | 1:B:101:HIS:CA | 1:B:101:HIS:C | 5        | 10.9          |
| (1,150) | 1:B:100:VAL:C | 1:B:101:HIS:N  | 1:B:101:HIS:CA | 1:B:101:HIS:C | 7        | 10.9          |
| (1,55)  | 1:A:112:GLY:C | 1:A:113:PHE:N  | 1:A:113:PHE:CA | 1:A:113:PHE:C | 5        | 10.7          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,35)  | 1:A:99:GLU:C  | 1:A:100:VAL:N  | 1:A:100:VAL:CA | 1:A:100:VAL:C | 7        | 10.7          |
| (1,154) | 1:B:102:GLY:C | 1:B:103:LYS:N  | 1:B:103:LYS:CA | 1:B:103:LYS:C | 1        | 10.7          |
| (1,91)  | 1:A:134:THR:N | 1:A:134:THR:CA | 1:A:134:THR:C  | 1:A:135:SER:N | 6        | 10.6          |
| (1,41)  | 1:A:102:GLY:C | 1:A:103:LYS:N  | 1:A:103:LYS:CA | 1:A:103:LYS:C | 1        | 10.6          |
| (1,204) | 1:B:134:THR:N | 1:B:134:THR:CA | 1:B:134:THR:C  | 1:B:135:SER:N | 6        | 10.6          |
| (1,148) | 1:B:99:GLU:C  | 1:B:100:VAL:N  | 1:B:100:VAL:CA | 1:B:100:VAL:C | 7        | 10.6          |
| (1,34)  | 1:A:99:GLU:N  | 1:A:99:GLU:CA  | 1:A:99:GLU:C   | 1:A:100:VAL:N | 3        | 10.5          |
| (1,168) | 1:B:112:GLY:C | 1:B:113:PHE:N  | 1:B:113:PHE:CA | 1:B:113:PHE:C | 5        | 10.5          |
| (1,12)  | 1:A:80:ASP:N  | 1:A:80:ASP:CA  | 1:A:80:ASP:C   | 1:A:81:VAL:N  | 8        | 10.5          |
| (1,32)  | 1:A:98:ILE:N  | 1:A:98:ILE:CA  | 1:A:98:ILE:C   | 1:A:99:GLU:N  | 5        | 10.4          |
| (1,147) | 1:B:99:GLU:N  | 1:B:99:GLU:CA  | 1:B:99:GLU:C   | 1:B:100:VAL:N | 3        | 10.4          |
| (1,130) | 1:B:88:GLU:C  | 1:B:89:LEU:N   | 1:B:89:LEU:CA  | 1:B:89:LEU:C  | 4        | 10.4          |
| (1,226) | 1:B:146:ASP:N | 1:B:146:ASP:CA | 1:B:146:ASP:C  | 1:B:147:GLY:N | 8        | 10.3          |
| (1,189) | 1:B:123:ARG:N | 1:B:123:ARG:CA | 1:B:123:ARG:C  | 1:B:124:ILE:N | 1        | 10.3          |
| (1,17)  | 1:A:88:GLU:C  | 1:A:89:LEU:N   | 1:A:89:LEU:CA  | 1:A:89:LEU:C  | 4        | 10.3          |
| (1,145) | 1:B:98:ILE:N  | 1:B:98:ILE:CA  | 1:B:98:ILE:C   | 1:B:99:GLU:N  | 5        | 10.3          |
| (1,125) | 1:B:80:ASP:N  | 1:B:80:ASP:CA  | 1:B:80:ASP:C   | 1:B:81:VAL:N  | 8        | 10.3          |
| (1,113) | 1:A:146:ASP:N | 1:A:146:ASP:CA | 1:A:146:ASP:C  | 1:A:147:GLY:N | 8        | 10.3          |
| (1,76)  | 1:A:123:ARG:N | 1:A:123:ARG:CA | 1:A:123:ARG:C  | 1:A:124:ILE:N | 1        | 10.2          |
| (1,32)  | 1:A:98:ILE:N  | 1:A:98:ILE:CA  | 1:A:98:ILE:C   | 1:A:99:GLU:N  | 4        | 10.1          |
| (1,145) | 1:B:98:ILE:N  | 1:B:98:ILE:CA  | 1:B:98:ILE:C   | 1:B:99:GLU:N  | 4        | 10.1          |
| (1,73)  | 1:A:121:LYS:C | 1:A:122:TYR:N  | 1:A:122:TYR:CA | 1:A:122:TYR:C | 5        | 9.8           |
| (1,35)  | 1:A:99:GLU:C  | 1:A:100:VAL:N  | 1:A:100:VAL:CA | 1:A:100:VAL:C | 4        | 9.6           |
| (1,21)  | 1:A:90:LYS:C  | 1:A:91:VAL:N   | 1:A:91:VAL:CA  | 1:A:91:VAL:C  | 5        | 9.6           |
| (1,186) | 1:B:121:LYS:C | 1:B:122:TYR:N  | 1:B:122:TYR:CA | 1:B:122:TYR:C | 5        | 9.6           |
| (1,148) | 1:B:99:GLU:C  | 1:B:100:VAL:N  | 1:B:100:VAL:CA | 1:B:100:VAL:C | 4        | 9.6           |
| (1,134) | 1:B:90:LYS:C  | 1:B:91:VAL:N   | 1:B:91:VAL:CA  | 1:B:91:VAL:C  | 5        | 9.6           |
| (1,24)  | 1:A:92:LYS:N  | 1:A:92:LYS:CA  | 1:A:92:LYS:C   | 1:A:93:VAL:N  | 4        | 9.3           |
| (1,66)  | 1:A:118:PHE:N | 1:A:118:PHE:CA | 1:A:118:PHE:C  | 1:A:119:HIS:N | 8        | 9.2           |
| (1,40)  | 1:A:102:GLY:N | 1:A:102:GLY:CA | 1:A:102:GLY:C  | 1:A:103:LYS:N | 2        | 9.2           |
| (1,22)  | 1:A:91:VAL:N  | 1:A:91:VAL:CA  | 1:A:91:VAL:C   | 1:A:92:LYS:N  | 1        | 9.2           |
| (1,137) | 1:B:92:LYS:N  | 1:B:92:LYS:CA  | 1:B:92:LYS:C   | 1:B:93:VAL:N  | 4        | 9.2           |
| (1,135) | 1:B:91:VAL:N  | 1:B:91:VAL:CA  | 1:B:91:VAL:C   | 1:B:92:LYS:N  | 1        | 9.2           |
| (1,179) | 1:B:118:PHE:N | 1:B:118:PHE:CA | 1:B:118:PHE:C  | 1:B:119:HIS:N | 8        | 9.1           |
| (1,154) | 1:B:102:GLY:C | 1:B:103:LYS:N  | 1:B:103:LYS:CA | 1:B:103:LYS:C | 6        | 9.1           |
| (1,153) | 1:B:102:GLY:N | 1:B:102:GLY:CA | 1:B:102:GLY:C  | 1:B:103:LYS:N | 2        | 9.1           |
| (1,41)  | 1:A:102:GLY:C | 1:A:103:LYS:N  | 1:A:103:LYS:CA | 1:A:103:LYS:C | 6        | 9.0           |
| (1,60)  | 1:A:115:SER:N | 1:A:115:SER:CA | 1:A:115:SER:C  | 1:A:116:ARG:N | 6        | 8.9           |
| (1,37)  | 1:A:100:VAL:C | 1:A:101:HIS:N  | 1:A:101:HIS:CA | 1:A:101:HIS:C | 6        | 8.8           |
| (1,36)  | 1:A:100:VAL:N | 1:A:100:VAL:CA | 1:A:100:VAL:C  | 1:A:101:HIS:N | 3        | 8.8           |
| (1,173) | 1:B:115:SER:N | 1:B:115:SER:CA | 1:B:115:SER:C  | 1:B:116:ARG:N | 6        | 8.8           |
| (1,150) | 1:B:100:VAL:C | 1:B:101:HIS:N  | 1:B:101:HIS:CA | 1:B:101:HIS:C | 6        | 8.8           |
| (1,149) | 1:B:100:VAL:N | 1:B:100:VAL:CA | 1:B:100:VAL:C  | 1:B:101:HIS:N | 3        | 8.8           |
| (1,6)   | 1:A:77:VAL:N  | 1:A:77:VAL:CA  | 1:A:77:VAL:C   | 1:A:78:ASN:N  | 6        | 8.7           |
| (1,41)  | 1:A:102:GLY:C | 1:A:103:LYS:N  | 1:A:103:LYS:CA | 1:A:103:LYS:C | 9        | 8.7           |
| (1,204) | 1:B:134:THR:N | 1:B:134:THR:CA | 1:B:134:THR:C  | 1:B:135:SER:N | 8        | 8.7           |
| (1,13)  | 1:A:83:HIS:C  | 1:A:84:PHE:N   | 1:A:84:PHE:CA  | 1:A:84:PHE:C  | 5        | 8.7           |
| (1,126) | 1:B:83:HIS:C  | 1:B:84:PHE:N   | 1:B:84:PHE:CA  | 1:B:84:PHE:C  | 5        | 8.7           |
| (1,91)  | 1:A:134:THR:N | 1:A:134:THR:CA | 1:A:134:THR:C  | 1:A:135:SER:N | 8        | 8.6           |
| (1,63)  | 1:A:116:ARG:C | 1:A:117:GLU:N  | 1:A:117:GLU:CA | 1:A:117:GLU:C | 2        | 8.6           |
| (1,154) | 1:B:102:GLY:C | 1:B:103:LYS:N  | 1:B:103:LYS:CA | 1:B:103:LYS:C | 9        | 8.6           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,119) | 1:B:77:VAL:N  | 1:B:77:VAL:CA  | 1:B:77:VAL:C   | 1:B:78:ASN:N  | 6        | 8.6           |
| (1,18)  | 1:A:89:LEU:N  | 1:A:89:LEU:CA  | 1:A:89:LEU:C   | 1:A:90:LYS:N  | 2        | 8.5           |
| (1,176) | 1:B:116:ARG:C | 1:B:117:GLU:N  | 1:B:117:GLU:CA | 1:B:117:GLU:C | 2        | 8.5           |
| (1,131) | 1:B:89:LEU:N  | 1:B:89:LEU:CA  | 1:B:89:LEU:C   | 1:B:90:LYS:N  | 2        | 8.5           |
| (1,51)  | 1:A:107:ARG:C | 1:A:108:GLN:N  | 1:A:108:GLN:CA | 1:A:108:GLN:C | 5        | 8.4           |
| (1,35)  | 1:A:99:GLU:C  | 1:A:100:VAL:N  | 1:A:100:VAL:CA | 1:A:100:VAL:C | 1        | 8.4           |
| (1,163) | 1:B:107:ARG:N | 1:B:107:ARG:CA | 1:B:107:ARG:C  | 1:B:108:GLN:N | 3        | 8.4           |
| (1,148) | 1:B:99:GLU:C  | 1:B:100:VAL:N  | 1:B:100:VAL:CA | 1:B:100:VAL:C | 1        | 8.4           |
| (1,58)  | 1:A:114:ILE:N | 1:A:114:ILE:CA | 1:A:114:ILE:C  | 1:A:115:SER:N | 9        | 8.3           |
| (1,32)  | 1:A:98:ILE:N  | 1:A:98:ILE:CA  | 1:A:98:ILE:C   | 1:A:99:GLU:N  | 2        | 8.3           |
| (1,171) | 1:B:114:ILE:N | 1:B:114:ILE:CA | 1:B:114:ILE:C  | 1:B:115:SER:N | 9        | 8.3           |
| (1,164) | 1:B:107:ARG:C | 1:B:108:GLN:N  | 1:B:108:GLN:CA | 1:B:108:GLN:C | 5        | 8.3           |
| (1,148) | 1:B:99:GLU:C  | 1:B:100:VAL:N  | 1:B:100:VAL:CA | 1:B:100:VAL:C | 9        | 8.3           |
| (1,50)  | 1:A:107:ARG:N | 1:A:107:ARG:CA | 1:A:107:ARG:C  | 1:A:108:GLN:N | 3        | 8.2           |
| (1,35)  | 1:A:99:GLU:C  | 1:A:100:VAL:N  | 1:A:100:VAL:CA | 1:A:100:VAL:C | 9        | 8.2           |
| (1,145) | 1:B:98:ILE:N  | 1:B:98:ILE:CA  | 1:B:98:ILE:C   | 1:B:99:GLU:N  | 2        | 8.2           |
| (1,61)  | 1:A:115:SER:C | 1:A:116:ARG:N  | 1:A:116:ARG:CA | 1:A:116:ARG:C | 5        | 8.1           |
| (1,174) | 1:B:115:SER:C | 1:B:116:ARG:N  | 1:B:116:ARG:CA | 1:B:116:ARG:C | 5        | 8.1           |
| (1,125) | 1:B:80:ASP:N  | 1:B:80:ASP:CA  | 1:B:80:ASP:C   | 1:B:81:VAL:N  | 3        | 8.0           |
| (1,12)  | 1:A:80:ASP:N  | 1:A:80:ASP:CA  | 1:A:80:ASP:C   | 1:A:81:VAL:N  | 3        | 8.0           |
| (1,26)  | 1:A:93:VAL:N  | 1:A:93:VAL:CA  | 1:A:93:VAL:C   | 1:A:94:LEU:N  | 8        | 7.9           |
| (1,139) | 1:B:93:VAL:N  | 1:B:93:VAL:CA  | 1:B:93:VAL:C   | 1:B:94:LEU:N  | 8        | 7.9           |
| (1,25)  | 1:A:92:LYS:C  | 1:A:93:VAL:N   | 1:A:93:VAL:CA  | 1:A:93:VAL:C  | 9        | 7.8           |
| (1,138) | 1:B:92:LYS:C  | 1:B:93:VAL:N   | 1:B:93:VAL:CA  | 1:B:93:VAL:C  | 9        | 7.8           |
| (1,25)  | 1:A:92:LYS:C  | 1:A:93:VAL:N   | 1:A:93:VAL:CA  | 1:A:93:VAL:C  | 1        | 7.7           |
| (1,182) | 1:B:119:HIS:C | 1:B:120:ARG:N  | 1:B:120:ARG:CA | 1:B:120:ARG:C | 8        | 7.6           |
| (1,138) | 1:B:92:LYS:C  | 1:B:93:VAL:N   | 1:B:93:VAL:CA  | 1:B:93:VAL:C  | 1        | 7.6           |
| (1,6)   | 1:A:77:VAL:N  | 1:A:77:VAL:CA  | 1:A:77:VAL:C   | 1:A:78:ASN:N  | 4        | 7.5           |
| (1,70)  | 1:A:120:ARG:N | 1:A:120:ARG:CA | 1:A:120:ARG:C  | 1:A:121:LYS:N | 6        | 7.4           |
| (1,69)  | 1:A:119:HIS:C | 1:A:120:ARG:N  | 1:A:120:ARG:CA | 1:A:120:ARG:C | 8        | 7.4           |
| (1,183) | 1:B:120:ARG:N | 1:B:120:ARG:CA | 1:B:120:ARG:C  | 1:B:121:LYS:N | 6        | 7.4           |
| (1,119) | 1:B:77:VAL:N  | 1:B:77:VAL:CA  | 1:B:77:VAL:C   | 1:B:78:ASN:N  | 4        | 7.4           |
| (1,85)  | 1:A:130:PRO:N | 1:A:130:PRO:CA | 1:A:130:PRO:C  | 1:A:131:LEU:N | 3        | 7.3           |
| (1,66)  | 1:A:118:PHE:N | 1:A:118:PHE:CA | 1:A:118:PHE:C  | 1:A:119:HIS:N | 5        | 7.3           |
| (1,179) | 1:B:118:PHE:N | 1:B:118:PHE:CA | 1:B:118:PHE:C  | 1:B:119:HIS:N | 5        | 7.3           |
| (1,153) | 1:B:102:GLY:N | 1:B:102:GLY:CA | 1:B:102:GLY:C  | 1:B:103:LYS:N | 7        | 7.3           |
| (1,148) | 1:B:99:GLU:C  | 1:B:100:VAL:N  | 1:B:100:VAL:CA | 1:B:100:VAL:C | 6        | 7.3           |
| (1,40)  | 1:A:102:GLY:N | 1:A:102:GLY:CA | 1:A:102:GLY:C  | 1:A:103:LYS:N | 7        | 7.2           |
| (1,35)  | 1:A:99:GLU:C  | 1:A:100:VAL:N  | 1:A:100:VAL:CA | 1:A:100:VAL:C | 6        | 7.2           |
| (1,198) | 1:B:130:PRO:N | 1:B:130:PRO:CA | 1:B:130:PRO:C  | 1:B:131:LEU:N | 3        | 7.2           |
| (1,140) | 1:B:93:VAL:C  | 1:B:94:LEU:N   | 1:B:94:LEU:CA  | 1:B:94:LEU:C  | 9        | 7.2           |
| (1,27)  | 1:A:93:VAL:C  | 1:A:94:LEU:N   | 1:A:94:LEU:CA  | 1:A:94:LEU:C  | 9        | 7.1           |
| (1,114) | 1:B:74:ARG:C  | 1:B:75:PHE:N   | 1:B:75:PHE:CA  | 1:B:75:PHE:C  | 9        | 7.1           |
| (1,1)   | 1:A:74:ARG:C  | 1:A:75:PHE:N   | 1:A:75:PHE:CA  | 1:A:75:PHE:C  | 9        | 7.1           |
| (1,8)   | 1:A:78:ASN:N  | 1:A:78:ASN:CA  | 1:A:78:ASN:C   | 1:A:79:LEU:N  | 2        | 6.6           |
| (1,61)  | 1:A:115:SER:C | 1:A:116:ARG:N  | 1:A:116:ARG:CA | 1:A:116:ARG:C | 2        | 6.6           |
| (1,6)   | 1:A:77:VAL:N  | 1:A:77:VAL:CA  | 1:A:77:VAL:C   | 1:A:78:ASN:N  | 8        | 6.6           |
| (1,185) | 1:B:121:LYS:N | 1:B:121:LYS:CA | 1:B:121:LYS:C  | 1:B:122:TYR:N | 9        | 6.6           |
| (1,174) | 1:B:115:SER:C | 1:B:116:ARG:N  | 1:B:116:ARG:CA | 1:B:116:ARG:C | 2        | 6.6           |
| (1,121) | 1:B:78:ASN:N  | 1:B:78:ASN:CA  | 1:B:78:ASN:C   | 1:B:79:LEU:N  | 2        | 6.6           |
| (1,72)  | 1:A:121:LYS:N | 1:A:121:LYS:CA | 1:A:121:LYS:C  | 1:A:122:TYR:N | 9        | 6.5           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,51)  | 1:A:107:ARG:C | 1:A:108:GLN:N  | 1:A:108:GLN:CA | 1:A:108:GLN:C | 8        | 6.5           |
| (1,183) | 1:B:120:ARG:N | 1:B:120:ARG:CA | 1:B:120:ARG:C  | 1:B:121:LYS:N | 4        | 6.5           |
| (1,119) | 1:B:77:VAL:N  | 1:B:77:VAL:CA  | 1:B:77:VAL:C   | 1:B:78:ASN:N  | 8        | 6.5           |
| (1,91)  | 1:A:134:THR:N | 1:A:134:THR:CA | 1:A:134:THR:C  | 1:A:135:SER:N | 1        | 6.4           |
| (1,72)  | 1:A:121:LYS:N | 1:A:121:LYS:CA | 1:A:121:LYS:C  | 1:A:122:TYR:N | 5        | 6.4           |
| (1,70)  | 1:A:120:ARG:N | 1:A:120:ARG:CA | 1:A:120:ARG:C  | 1:A:121:LYS:N | 4        | 6.4           |
| (1,21)  | 1:A:90:LYS:C  | 1:A:91:VAL:N   | 1:A:91:VAL:CA  | 1:A:91:VAL:C  | 9        | 6.4           |
| (1,204) | 1:B:134:THR:N | 1:B:134:THR:CA | 1:B:134:THR:C  | 1:B:135:SER:N | 1        | 6.4           |
| (1,164) | 1:B:107:ARG:C | 1:B:108:GLN:N  | 1:B:108:GLN:CA | 1:B:108:GLN:C | 8        | 6.4           |
| (1,185) | 1:B:121:LYS:N | 1:B:121:LYS:CA | 1:B:121:LYS:C  | 1:B:122:TYR:N | 3        | 6.3           |
| (1,134) | 1:B:90:LYS:C  | 1:B:91:VAL:N   | 1:B:91:VAL:CA  | 1:B:91:VAL:C  | 9        | 6.3           |
| (1,72)  | 1:A:121:LYS:N | 1:A:121:LYS:CA | 1:A:121:LYS:C  | 1:A:122:TYR:N | 3        | 6.2           |
| (1,185) | 1:B:121:LYS:N | 1:B:121:LYS:CA | 1:B:121:LYS:C  | 1:B:122:TYR:N | 5        | 6.2           |
| (1,53)  | 1:A:110:GLU:C | 1:A:111:HIS:N  | 1:A:111:HIS:CA | 1:A:111:HIS:C | 2        | 6.0           |
| (1,42)  | 1:A:103:LYS:N | 1:A:103:LYS:CA | 1:A:103:LYS:C  | 1:A:104:HIS:N | 5        | 6.0           |
| (1,166) | 1:B:110:GLU:C | 1:B:111:HIS:N  | 1:B:111:HIS:CA | 1:B:111:HIS:C | 2        | 6.0           |
| (1,155) | 1:B:103:LYS:N | 1:B:103:LYS:CA | 1:B:103:LYS:C  | 1:B:104:HIS:N | 5        | 6.0           |
| (1,69)  | 1:A:119:HIS:C | 1:A:120:ARG:N  | 1:A:120:ARG:CA | 1:A:120:ARG:C | 4        | 5.9           |
| (1,41)  | 1:A:102:GLY:C | 1:A:103:LYS:N  | 1:A:103:LYS:CA | 1:A:103:LYS:C | 5        | 5.9           |
| (1,21)  | 1:A:90:LYS:C  | 1:A:91:VAL:N   | 1:A:91:VAL:CA  | 1:A:91:VAL:C  | 3        | 5.9           |
| (1,182) | 1:B:119:HIS:C | 1:B:120:ARG:N  | 1:B:120:ARG:CA | 1:B:120:ARG:C | 4        | 5.9           |
| (1,134) | 1:B:90:LYS:C  | 1:B:91:VAL:N   | 1:B:91:VAL:CA  | 1:B:91:VAL:C  | 3        | 5.9           |
| (1,163) | 1:B:107:ARG:N | 1:B:107:ARG:CA | 1:B:107:ARG:C  | 1:B:108:GLN:N | 9        | 5.8           |
| (1,154) | 1:B:102:GLY:C | 1:B:103:LYS:N  | 1:B:103:LYS:CA | 1:B:103:LYS:C | 5        | 5.8           |
| (1,138) | 1:B:92:LYS:C  | 1:B:93:VAL:N   | 1:B:93:VAL:CA  | 1:B:93:VAL:C  | 3        | 5.8           |
| (1,8)   | 1:A:78:ASN:N  | 1:A:78:ASN:CA  | 1:A:78:ASN:C   | 1:A:79:LEU:N  | 8        | 5.7           |
| (1,50)  | 1:A:107:ARG:N | 1:A:107:ARG:CA | 1:A:107:ARG:C  | 1:A:108:GLN:N | 9        | 5.7           |
| (1,25)  | 1:A:92:LYS:C  | 1:A:93:VAL:N   | 1:A:93:VAL:CA  | 1:A:93:VAL:C  | 3        | 5.7           |
| (1,121) | 1:B:78:ASN:N  | 1:B:78:ASN:CA  | 1:B:78:ASN:C   | 1:B:79:LEU:N  | 8        | 5.7           |
| (1,176) | 1:B:116:ARG:C | 1:B:117:GLU:N  | 1:B:117:GLU:CA | 1:B:117:GLU:C | 4        | 5.6           |
| (1,63)  | 1:A:116:ARG:C | 1:A:117:GLU:N  | 1:A:117:GLU:CA | 1:A:117:GLU:C | 4        | 5.5           |
| (1,174) | 1:B:115:SER:C | 1:B:116:ARG:N  | 1:B:116:ARG:CA | 1:B:116:ARG:C | 3        | 5.5           |
| (1,113) | 1:A:146:ASP:N | 1:A:146:ASP:CA | 1:A:146:ASP:C  | 1:A:147:GLY:N | 7        | 5.5           |
| (1,61)  | 1:A:115:SER:C | 1:A:116:ARG:N  | 1:A:116:ARG:CA | 1:A:116:ARG:C | 3        | 5.4           |
| (1,226) | 1:B:146:ASP:N | 1:B:146:ASP:CA | 1:B:146:ASP:C  | 1:B:147:GLY:N | 7        | 5.4           |
| (1,124) | 1:B:79:LEU:C  | 1:B:80:ASP:N   | 1:B:80:ASP:CA  | 1:B:80:ASP:C  | 3        | 5.4           |
| (1,11)  | 1:A:79:LEU:C  | 1:A:80:ASP:N   | 1:A:80:ASP:CA  | 1:A:80:ASP:C  | 3        | 5.4           |
| (1,51)  | 1:A:107:ARG:C | 1:A:108:GLN:N  | 1:A:108:GLN:CA | 1:A:108:GLN:C | 7        | 5.3           |
| (1,164) | 1:B:107:ARG:C | 1:B:108:GLN:N  | 1:B:108:GLN:CA | 1:B:108:GLN:C | 7        | 5.3           |
| (1,59)  | 1:A:114:ILE:C | 1:A:115:SER:N  | 1:A:115:SER:CA | 1:A:115:SER:C | 4        | 5.1           |
| (1,35)  | 1:A:99:GLU:C  | 1:A:100:VAL:N  | 1:A:100:VAL:CA | 1:A:100:VAL:C | 3        | 5.1           |
| (1,172) | 1:B:114:ILE:C | 1:B:115:SER:N  | 1:B:115:SER:CA | 1:B:115:SER:C | 4        | 5.1           |
| (1,148) | 1:B:99:GLU:C  | 1:B:100:VAL:N  | 1:B:100:VAL:CA | 1:B:100:VAL:C | 3        | 5.1           |
| (1,224) | 1:B:145:VAL:N | 1:B:145:VAL:CA | 1:B:145:VAL:C  | 1:B:146:ASP:N | 1        | 4.9           |
| (1,111) | 1:A:145:VAL:N | 1:A:145:VAL:CA | 1:A:145:VAL:C  | 1:A:146:ASP:N | 1        | 4.9           |
| (1,91)  | 1:A:134:THR:N | 1:A:134:THR:CA | 1:A:134:THR:C  | 1:A:135:SER:N | 5        | 4.8           |
| (1,20)  | 1:A:90:LYS:N  | 1:A:90:LYS:CA  | 1:A:90:LYS:C   | 1:A:91:VAL:N  | 5        | 4.8           |
| (1,204) | 1:B:134:THR:N | 1:B:134:THR:CA | 1:B:134:THR:C  | 1:B:135:SER:N | 5        | 4.7           |
| (1,199) | 1:B:131:LEU:C | 1:B:132:THR:N  | 1:B:132:THR:CA | 1:B:132:THR:C | 8        | 4.7           |
| (1,133) | 1:B:90:LYS:N  | 1:B:90:LYS:CA  | 1:B:90:LYS:C   | 1:B:91:VAL:N  | 5        | 4.7           |
| (1,99)  | 1:A:138:SER:N | 1:A:138:SER:CA | 1:A:138:SER:C  | 1:A:139:SER:N | 4        | 4.6           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,86)  | 1:A:131:LEU:C | 1:A:132:THR:N  | 1:A:132:THR:CA | 1:A:132:THR:C | 8        | 4.6           |
| (1,19)  | 1:A:89:LEU:C  | 1:A:90:LYS:N   | 1:A:90:LYS:CA  | 1:A:90:LYS:C  | 9        | 4.6           |
| (1,132) | 1:B:89:LEU:C  | 1:B:90:LYS:N   | 1:B:90:LYS:CA  | 1:B:90:LYS:C  | 9        | 4.6           |
| (1,51)  | 1:A:107:ARG:C | 1:A:108:GLN:N  | 1:A:108:GLN:CA | 1:A:108:GLN:C | 1        | 4.5           |
| (1,27)  | 1:A:93:VAL:C  | 1:A:94:LEU:N   | 1:A:94:LEU:CA  | 1:A:94:LEU:C  | 4        | 4.5           |
| (1,212) | 1:B:138:SER:N | 1:B:138:SER:CA | 1:B:138:SER:C  | 1:B:139:SER:N | 4        | 4.5           |
| (1,140) | 1:B:93:VAL:C  | 1:B:94:LEU:N   | 1:B:94:LEU:CA  | 1:B:94:LEU:C  | 4        | 4.5           |
| (1,164) | 1:B:107:ARG:C | 1:B:108:GLN:N  | 1:B:108:GLN:CA | 1:B:108:GLN:C | 1        | 4.4           |
| (1,124) | 1:B:79:LEU:C  | 1:B:80:ASP:N   | 1:B:80:ASP:CA  | 1:B:80:ASP:C  | 2        | 4.4           |
| (1,122) | 1:B:78:ASN:C  | 1:B:79:LEU:N   | 1:B:79:LEU:CA  | 1:B:79:LEU:C  | 8        | 4.4           |
| (1,11)  | 1:A:79:LEU:C  | 1:A:80:ASP:N   | 1:A:80:ASP:CA  | 1:A:80:ASP:C  | 2        | 4.4           |
| (1,9)   | 1:A:78:ASN:C  | 1:A:79:LEU:N   | 1:A:79:LEU:CA  | 1:A:79:LEU:C  | 8        | 4.3           |
| (1,72)  | 1:A:121:LYS:N | 1:A:121:LYS:CA | 1:A:121:LYS:C  | 1:A:122:TYR:N | 4        | 4.2           |
| (1,62)  | 1:A:116:ARG:N | 1:A:116:ARG:CA | 1:A:116:ARG:C  | 1:A:117:GLU:N | 9        | 4.2           |
| (1,175) | 1:B:116:ARG:N | 1:B:116:ARG:CA | 1:B:116:ARG:C  | 1:B:117:GLU:N | 9        | 4.2           |
| (1,185) | 1:B:121:LYS:N | 1:B:121:LYS:CA | 1:B:121:LYS:C  | 1:B:122:TYR:N | 4        | 4.1           |
| (1,55)  | 1:A:112:GLY:C | 1:A:113:PHE:N  | 1:A:113:PHE:CA | 1:A:113:PHE:C | 6        | 4.0           |
| (1,27)  | 1:A:93:VAL:C  | 1:A:94:LEU:N   | 1:A:94:LEU:CA  | 1:A:94:LEU:C  | 7        | 4.0           |
| (1,168) | 1:B:112:GLY:C | 1:B:113:PHE:N  | 1:B:113:PHE:CA | 1:B:113:PHE:C | 6        | 4.0           |
| (1,140) | 1:B:93:VAL:C  | 1:B:94:LEU:N   | 1:B:94:LEU:CA  | 1:B:94:LEU:C  | 7        | 4.0           |
| (1,4)   | 1:A:76:SER:N  | 1:A:76:SER:CA  | 1:A:76:SER:C   | 1:A:77:VAL:N  | 6        | 3.9           |
| (1,117) | 1:B:76:SER:N  | 1:B:76:SER:CA  | 1:B:76:SER:C   | 1:B:77:VAL:N  | 6        | 3.9           |
| (1,116) | 1:B:75:PHE:C  | 1:B:76:SER:N   | 1:B:76:SER:CA  | 1:B:76:SER:C  | 3        | 3.9           |
| (1,66)  | 1:A:118:PHE:N | 1:A:118:PHE:CA | 1:A:118:PHE:C  | 1:A:119:HIS:N | 1        | 3.8           |
| (1,3)   | 1:A:75:PHE:C  | 1:A:76:SER:N   | 1:A:76:SER:CA  | 1:A:76:SER:C  | 3        | 3.8           |
| (1,179) | 1:B:118:PHE:N | 1:B:118:PHE:CA | 1:B:118:PHE:C  | 1:B:119:HIS:N | 1        | 3.8           |
| (1,21)  | 1:A:90:LYS:C  | 1:A:91:VAL:N   | 1:A:91:VAL:CA  | 1:A:91:VAL:C  | 6        | 3.7           |
| (1,147) | 1:B:99:GLU:N  | 1:B:99:GLU:CA  | 1:B:99:GLU:C   | 1:B:100:VAL:N | 9        | 3.6           |
| (1,134) | 1:B:90:LYS:C  | 1:B:91:VAL:N   | 1:B:91:VAL:CA  | 1:B:91:VAL:C  | 6        | 3.6           |
| (1,34)  | 1:A:99:GLU:N  | 1:A:99:GLU:CA  | 1:A:99:GLU:C   | 1:A:100:VAL:N | 9        | 3.5           |
| (1,58)  | 1:A:114:ILE:N | 1:A:114:ILE:CA | 1:A:114:ILE:C  | 1:A:115:SER:N | 6        | 3.4           |
| (1,25)  | 1:A:92:LYS:C  | 1:A:93:VAL:N   | 1:A:93:VAL:CA  | 1:A:93:VAL:C  | 6        | 3.4           |
| (1,24)  | 1:A:92:LYS:N  | 1:A:92:LYS:CA  | 1:A:92:LYS:C   | 1:A:93:VAL:N  | 1        | 3.4           |
| (1,152) | 1:B:101:HIS:C | 1:B:102:GLY:N  | 1:B:102:GLY:CA | 1:B:102:GLY:C | 9        | 3.4           |
| (1,137) | 1:B:92:LYS:N  | 1:B:92:LYS:CA  | 1:B:92:LYS:C   | 1:B:93:VAL:N  | 1        | 3.4           |
| (1,70)  | 1:A:120:ARG:N | 1:A:120:ARG:CA | 1:A:120:ARG:C  | 1:A:121:LYS:N | 3        | 3.3           |
| (1,39)  | 1:A:101:HIS:C | 1:A:102:GLY:N  | 1:A:102:GLY:CA | 1:A:102:GLY:C | 9        | 3.3           |
| (1,171) | 1:B:114:ILE:N | 1:B:114:ILE:CA | 1:B:114:ILE:C  | 1:B:115:SER:N | 6        | 3.3           |
| (1,138) | 1:B:92:LYS:C  | 1:B:93:VAL:N   | 1:B:93:VAL:CA  | 1:B:93:VAL:C  | 6        | 3.3           |
| (1,222) | 1:B:144:THR:N | 1:B:144:THR:CA | 1:B:144:THR:C  | 1:B:145:VAL:N | 6        | 3.2           |
| (1,125) | 1:B:80:ASP:N  | 1:B:80:ASP:CA  | 1:B:80:ASP:C   | 1:B:81:VAL:N  | 7        | 3.2           |
| (1,12)  | 1:A:80:ASP:N  | 1:A:80:ASP:CA  | 1:A:80:ASP:C   | 1:A:81:VAL:N  | 7        | 3.2           |
| (1,92)  | 1:A:134:THR:C | 1:A:135:SER:N  | 1:A:135:SER:CA | 1:A:135:SER:C | 5        | 3.1           |
| (1,205) | 1:B:134:THR:C | 1:B:135:SER:N  | 1:B:135:SER:CA | 1:B:135:SER:C | 5        | 3.1           |
| (1,183) | 1:B:120:ARG:N | 1:B:120:ARG:CA | 1:B:120:ARG:C  | 1:B:121:LYS:N | 3        | 3.1           |
| (1,25)  | 1:A:92:LYS:C  | 1:A:93:VAL:N   | 1:A:93:VAL:CA  | 1:A:93:VAL:C  | 4        | 3.0           |
| (1,171) | 1:B:114:ILE:N | 1:B:114:ILE:CA | 1:B:114:ILE:C  | 1:B:115:SER:N | 8        | 3.0           |
| (1,109) | 1:A:144:THR:N | 1:A:144:THR:CA | 1:A:144:THR:C  | 1:A:145:VAL:N | 6        | 3.0           |
| (1,65)  | 1:A:117:GLU:C | 1:A:118:PHE:N  | 1:A:118:PHE:CA | 1:A:118:PHE:C | 9        | 2.9           |
| (1,58)  | 1:A:114:ILE:N | 1:A:114:ILE:CA | 1:A:114:ILE:C  | 1:A:115:SER:N | 8        | 2.9           |
| (1,138) | 1:B:92:LYS:C  | 1:B:93:VAL:N   | 1:B:93:VAL:CA  | 1:B:93:VAL:C  | 4        | 2.9           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,22)  | 1:A:91:VAL:N  | 1:A:91:VAL:CA  | 1:A:91:VAL:C   | 1:A:92:LYS:N  | 3        | 2.8           |
| (1,178) | 1:B:117:GLU:C | 1:B:118:PHE:N  | 1:B:118:PHE:CA | 1:B:118:PHE:C | 9        | 2.8           |
| (1,174) | 1:B:115:SER:C | 1:B:116:ARG:N  | 1:B:116:ARG:CA | 1:B:116:ARG:C | 1        | 2.8           |
| (1,135) | 1:B:91:VAL:N  | 1:B:91:VAL:CA  | 1:B:91:VAL:C   | 1:B:92:LYS:N  | 3        | 2.8           |
| (1,61)  | 1:A:115:SER:C | 1:A:116:ARG:N  | 1:A:116:ARG:CA | 1:A:116:ARG:C | 1        | 2.7           |
| (1,58)  | 1:A:114:ILE:N | 1:A:114:ILE:CA | 1:A:114:ILE:C  | 1:A:115:SER:N | 3        | 2.7           |
| (1,171) | 1:B:114:ILE:N | 1:B:114:ILE:CA | 1:B:114:ILE:C  | 1:B:115:SER:N | 3        | 2.7           |
| (1,8)   | 1:A:78:ASN:N  | 1:A:78:ASN:CA  | 1:A:78:ASN:C   | 1:A:79:LEU:N  | 9        | 2.6           |
| (1,57)  | 1:A:113:PHE:C | 1:A:114:ILE:N  | 1:A:114:ILE:CA | 1:A:114:ILE:C | 9        | 2.6           |
| (1,55)  | 1:A:112:GLY:C | 1:A:113:PHE:N  | 1:A:113:PHE:CA | 1:A:113:PHE:C | 3        | 2.6           |
| (1,168) | 1:B:112:GLY:C | 1:B:113:PHE:N  | 1:B:113:PHE:CA | 1:B:113:PHE:C | 3        | 2.6           |
| (1,121) | 1:B:78:ASN:N  | 1:B:78:ASN:CA  | 1:B:78:ASN:C   | 1:B:79:LEU:N  | 9        | 2.6           |
| (1,7)   | 1:A:77:VAL:C  | 1:A:78:ASN:N   | 1:A:78:ASN:CA  | 1:A:78:ASN:C  | 4        | 2.5           |
| (1,170) | 1:B:113:PHE:C | 1:B:114:ILE:N  | 1:B:114:ILE:CA | 1:B:114:ILE:C | 9        | 2.5           |
| (1,118) | 1:B:76:SER:C  | 1:B:77:VAL:N   | 1:B:77:VAL:CA  | 1:B:77:VAL:C  | 4        | 2.5           |
| (1,80)  | 1:A:126:ALA:N | 1:A:126:ALA:CA | 1:A:126:ALA:C  | 1:A:127:ASP:N | 4        | 2.4           |
| (1,5)   | 1:A:76:SER:C  | 1:A:77:VAL:N   | 1:A:77:VAL:CA  | 1:A:77:VAL:C  | 4        | 2.4           |
| (1,193) | 1:B:126:ALA:N | 1:B:126:ALA:CA | 1:B:126:ALA:C  | 1:B:127:ASP:N | 4        | 2.4           |
| (1,120) | 1:B:77:VAL:C  | 1:B:78:ASN:N   | 1:B:78:ASN:CA  | 1:B:78:ASN:C  | 4        | 2.4           |
| (1,25)  | 1:A:92:LYS:C  | 1:A:93:VAL:N   | 1:A:93:VAL:CA  | 1:A:93:VAL:C  | 7        | 2.3           |
| (1,125) | 1:B:80:ASP:N  | 1:B:80:ASP:CA  | 1:B:80:ASP:C   | 1:B:81:VAL:N  | 6        | 2.3           |
| (1,12)  | 1:A:80:ASP:N  | 1:A:80:ASP:CA  | 1:A:80:ASP:C   | 1:A:81:VAL:N  | 6        | 2.3           |
| (1,138) | 1:B:92:LYS:C  | 1:B:93:VAL:N   | 1:B:93:VAL:CA  | 1:B:93:VAL:C  | 7        | 2.2           |
| (1,69)  | 1:A:119:HIS:C | 1:A:120:ARG:N  | 1:A:120:ARG:CA | 1:A:120:ARG:C | 7        | 2.0           |
| (1,182) | 1:B:119:HIS:C | 1:B:120:ARG:N  | 1:B:120:ARG:CA | 1:B:120:ARG:C | 7        | 2.0           |
| (1,124) | 1:B:79:LEU:C  | 1:B:80:ASP:N   | 1:B:80:ASP:CA  | 1:B:80:ASP:C  | 9        | 2.0           |
| (1,11)  | 1:A:79:LEU:C  | 1:A:80:ASP:N   | 1:A:80:ASP:CA  | 1:A:80:ASP:C  | 9        | 2.0           |
| (1,93)  | 1:A:135:SER:N | 1:A:135:SER:CA | 1:A:135:SER:C  | 1:A:136:SER:N | 8        | 1.9           |
| (1,67)  | 1:A:118:PHE:C | 1:A:119:HIS:N  | 1:A:119:HIS:CA | 1:A:119:HIS:C | 4        | 1.9           |
| (1,226) | 1:B:146:ASP:N | 1:B:146:ASP:CA | 1:B:146:ASP:C  | 1:B:147:GLY:N | 5        | 1.9           |
| (1,113) | 1:A:146:ASP:N | 1:A:146:ASP:CA | 1:A:146:ASP:C  | 1:A:147:GLY:N | 5        | 1.9           |
| (1,5)   | 1:A:76:SER:C  | 1:A:77:VAL:N   | 1:A:77:VAL:CA  | 1:A:77:VAL:C  | 8        | 1.8           |
| (1,3)   | 1:A:75:PHE:C  | 1:A:76:SER:N   | 1:A:76:SER:CA  | 1:A:76:SER:C  | 2        | 1.8           |
| (1,27)  | 1:A:93:VAL:C  | 1:A:94:LEU:N   | 1:A:94:LEU:CA  | 1:A:94:LEU:C  | 5        | 1.8           |
| (1,206) | 1:B:135:SER:N | 1:B:135:SER:CA | 1:B:135:SER:C  | 1:B:136:SER:N | 8        | 1.8           |
| (1,180) | 1:B:118:PHE:C | 1:B:119:HIS:N  | 1:B:119:HIS:CA | 1:B:119:HIS:C | 4        | 1.8           |
| (1,125) | 1:B:80:ASP:N  | 1:B:80:ASP:CA  | 1:B:80:ASP:C   | 1:B:81:VAL:N  | 1        | 1.8           |
| (1,116) | 1:B:75:PHE:C  | 1:B:76:SER:N   | 1:B:76:SER:CA  | 1:B:76:SER:C  | 2        | 1.8           |
| (1,92)  | 1:A:134:THR:C | 1:A:135:SER:N  | 1:A:135:SER:CA | 1:A:135:SER:C | 6        | 1.7           |
| (1,205) | 1:B:134:THR:C | 1:B:135:SER:N  | 1:B:135:SER:CA | 1:B:135:SER:C | 6        | 1.7           |
| (1,186) | 1:B:121:LYS:C | 1:B:122:TYR:N  | 1:B:122:TYR:CA | 1:B:122:TYR:C | 4        | 1.7           |
| (1,140) | 1:B:93:VAL:C  | 1:B:94:LEU:N   | 1:B:94:LEU:CA  | 1:B:94:LEU:C  | 5        | 1.7           |
| (1,12)  | 1:A:80:ASP:N  | 1:A:80:ASP:CA  | 1:A:80:ASP:C   | 1:A:81:VAL:N  | 1        | 1.7           |
| (1,118) | 1:B:76:SER:C  | 1:B:77:VAL:N   | 1:B:77:VAL:CA  | 1:B:77:VAL:C  | 8        | 1.7           |
| (1,73)  | 1:A:121:LYS:C | 1:A:122:TYR:N  | 1:A:122:TYR:CA | 1:A:122:TYR:C | 4        | 1.6           |
| (1,176) | 1:B:116:ARG:C | 1:B:117:GLU:N  | 1:B:117:GLU:CA | 1:B:117:GLU:C | 6        | 1.6           |
| (1,63)  | 1:A:116:ARG:C | 1:A:117:GLU:N  | 1:A:117:GLU:CA | 1:A:117:GLU:C | 5        | 1.5           |
| (1,63)  | 1:A:116:ARG:C | 1:A:117:GLU:N  | 1:A:117:GLU:CA | 1:A:117:GLU:C | 6        | 1.5           |
| (1,135) | 1:B:91:VAL:N  | 1:B:91:VAL:CA  | 1:B:91:VAL:C   | 1:B:92:LYS:N  | 2        | 1.5           |
| (1,62)  | 1:A:116:ARG:N | 1:A:116:ARG:CA | 1:A:116:ARG:C  | 1:A:117:GLU:N | 7        | 1.4           |
| (1,22)  | 1:A:91:VAL:N  | 1:A:91:VAL:CA  | 1:A:91:VAL:C   | 1:A:92:LYS:N  | 2        | 1.4           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,176) | 1:B:116:ARG:C | 1:B:117:GLU:N  | 1:B:117:GLU:CA | 1:B:117:GLU:C | 5        | 1.4           |
| (1,175) | 1:B:116:ARG:N | 1:B:116:ARG:CA | 1:B:116:ARG:C  | 1:B:117:GLU:N | 7        | 1.4           |
| (1,61)  | 1:A:115:SER:C | 1:A:116:ARG:N  | 1:A:116:ARG:CA | 1:A:116:ARG:C | 8        | 1.3           |
| (1,125) | 1:B:80:ASP:N  | 1:B:80:ASP:CA  | 1:B:80:ASP:C   | 1:B:81:VAL:N  | 2        | 1.3           |
| (1,12)  | 1:A:80:ASP:N  | 1:A:80:ASP:CA  | 1:A:80:ASP:C   | 1:A:81:VAL:N  | 2        | 1.3           |
| (1,90)  | 1:A:133:ILE:C | 1:A:134:THR:N  | 1:A:134:THR:CA | 1:A:134:THR:C | 3        | 1.2           |
| (1,27)  | 1:A:93:VAL:C  | 1:A:94:LEU:N   | 1:A:94:LEU:CA  | 1:A:94:LEU:C  | 6        | 1.2           |
| (1,168) | 1:B:112:GLY:C | 1:B:113:PHE:N  | 1:B:113:PHE:CA | 1:B:113:PHE:C | 1        | 1.2           |
| (1,55)  | 1:A:112:GLY:C | 1:A:113:PHE:N  | 1:A:113:PHE:CA | 1:A:113:PHE:C | 1        | 1.1           |
| (1,224) | 1:B:145:VAL:N | 1:B:145:VAL:CA | 1:B:145:VAL:C  | 1:B:146:ASP:N | 8        | 1.1           |
| (1,203) | 1:B:133:ILE:C | 1:B:134:THR:N  | 1:B:134:THR:CA | 1:B:134:THR:C | 3        | 1.1           |
| (1,174) | 1:B:115:SER:C | 1:B:116:ARG:N  | 1:B:116:ARG:CA | 1:B:116:ARG:C | 8        | 1.1           |
| (1,140) | 1:B:93:VAL:C  | 1:B:94:LEU:N   | 1:B:94:LEU:CA  | 1:B:94:LEU:C  | 6        | 1.1           |